

New Characterizations of Matrix Φ -Entropies, Poincaré and Sobolev Inequalities and an Upper Bound to Holevo Quantity

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ABSTRACT. We derive new characterizations of the matrix Φ -entropies introduced in [*Electron. J. Probab.*, **19**(20): 1–30, 2014]. These characterizations help to better understand the properties of matrix Φ -entropies, and are a powerful tool for establishing matrix concentration inequalities for matrix-valued functions of independent random variables. In particular, we use the subadditivity property to prove a Poincaré inequality for the matrix Φ -entropies. We also provide a new proof for the matrix Efron-Stein inequality. Furthermore, we derive logarithmic Sobolev inequalities for matrix-valued functions defined on Boolean hypercubes and with Gaussian distributions. Our proof relies on the powerful matrix Bonami-Beckner inequality. Finally, the Holevo quantity in quantum information theory is closely related to the matrix Φ -entropies. This allows us to upper bound the Holevo quantity of a classical-quantum ensemble that undergoes a special Markov evolution.

1. INTRODUCTION

The introduction of classical Φ -entropies can be traced back to the early days of information theory, where the notion of ϕ -divergence [1] and convex analysis [2–4] is defined. Formally, classical Φ -entropies refer to the set of functions $\Phi : [0, \infty) \rightarrow \mathbb{R}$ that are continuous, convex on $[0, \infty)$, twice differentiable on $(0, \infty)$, and either Φ is affine or Φ'' is strictly positive and $1/\Phi''$ is concave. This set includes rich members, e.g. x^p , $p \in [1, 2]$, and $x \log x$. For every nonnegative integrable random variable Z , the Φ -entropy function H_Φ is defined as

$$H_\Phi(Z) = \mathbb{E}\Phi(Z) - \Phi(\mathbb{E}Z).$$

It can already be seen that the variance and the entropy function of Z correspond to $H_{x^2}(Z)$ and $H_{x \log x}(Z)$, respectively.

The investigation of the general properties of the Φ -entropies has enjoyed great success because it unifies the study of concentration inequalities [5]. Of these, the *subadditivity* property of the Φ -entropies has led to the derivation of Φ -Sobolev inequalities, generalizing the logarithmic Sobolev (i.e. log-Sobolev) and Poincaré inequalities, which in turn, is a crucial step toward the powerful Bousquet's inequality [6, 7]. Let $Z = f(X_1, \dots, X_n)$, where X_1, \dots, X_n are independent random variables, and f is a nonnegative function. We say $H_\Phi(Z)$ is *subadditive* if

$$H_\Phi(Z) \leq \sum_{i=1}^n \mathbb{E}H_\Phi^{(i)}(Z)$$

where $H_\Phi^{(i)}(Z) = \mathbb{E}_i\Phi(Z) - \Phi(\mathbb{E}_iZ)$ is the conditional entropy, and \mathbb{E}_i denotes conditional expectation conditioned on the $n-1$ random variables $X_{-i} \triangleq (X_1, \dots, X_{i-1}, X_{i+1}, \dots, X_n)$. The subadditivity property and the definition of Φ -entropies are intimately connected to each other. In fact, one can show that they are equivalent [8, 9]. Furthermore, more equivalent statements between the subadditivity of the classical

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Φ -entropies and convexity of other forms of the function Φ have also been established, which proves to be useful in other contexts as well [8, 9].

In many branches of science and engineering, observed data are more efficiently represented as matrices, and system performance can be concluded from analysis where random assumption is placed on the matrices. The subject of random matrices has undergone extensive studies, independently conducted in their own discipline, in the 20th century. A recent review of modern random matrix theory by Tropp surveyed the most successful methods from these areas, and provided interesting examples that these techniques can illuminate [10]. It is clear that the future development of random matrix theory will benefit from a unified and systematical treatment.

Parallel to the classical entropy method, Chen and Tropp defined the class of trace matrix Φ -entropies [11]. The class of matrix entropy functions can be equivalently characterised in terms of the second derivative of their representing function, and this equivalent statement easily guarantees that the set of matrix entropies is therefore a convex cone [12]. Consider a random matrix \mathbf{Z} taking values in \mathbb{M}_d^+ , with $\mathbb{E}\|\mathbf{Z}\|_\infty < \infty$ and $\mathbb{E}\|\Phi(\mathbf{Z})\|_\infty < \infty$. The matrix Φ -entropy functional H_Φ is defined as

$$H_\Phi(\mathbf{Z}) \triangleq \overline{\text{tr}}[\mathbb{E}\Phi(\mathbf{Z}) - \Phi(\mathbb{E}\mathbf{Z})],$$

where $\overline{\text{tr}}$ is the normalized trace [11]. The matrix Φ -entropies are subadditive. Unlike its classical counterpart, very little connection between the matrix Φ -entropies and other convex forms of the same functions in the class is established [12, 13].

In this paper, we prove new characterizations of the class of matrix Φ -entropies defined in [11]. Furthermore, our results show that matrix Φ -entropies satisfy all known equivalent statements that classical Φ -entropy functions satisfy [5, 8, 9]. Our results provide additional justification to its original definition of the matrix Φ -entropies, which is a matrix generalization of the classical Φ -entropies. The equivalences between matrix Φ -entropies and other convex forms of the function Φ will help to understand the class of entropy functions and to unify the study of matrix concentration inequalities in the future.

The study of log-Sobolev, Poincaré and hypercontractivity was originally motivated by the question of how fast a Markov process and Markov chain can mix, e.g., the mixing property. Interested readers can find detailed discussion in, e.g., Ref. [14]. The pioneering work by Gross in 1975 derived the log-Sobolev inequalities for the balanced Bernoulli and Gaussian distributions, and determined the optimal constant in the former case [15]. Bonami and Beckner independently discovered a version of hypercontractivity inequality. Since then, it has become a rich area of research that influences the investigation of, among others, a non-asymptotic theory of concentration inequalities.

Log-Sobolev and hypercontractivity have also emerged as a powerful tool in quantum information theory [16–23], and have found many applications [20]. In quantum field theory, hypercontractivity is used to prove tighter mixing time bounds in the analysis of certain physics systems whose evolutions can be modelled as continuous time Markov processes [16, 17, 21]. In theoretical computer science, hypercontractivity is used to bound the local influence of a binary bit to the total matrix-valued function [18, 19]. A remarkable step was made by King [22] who generalizes classical hypercontractivity for the boolean cube to non-commutative quantum hypercontractivity for the depolarizing channel.

We extend those studies of non-commutative Poincaré inequalities and log-Sobolev inequalities to the random matrix framework. In other words, we establish matrix concentration inequalities, such as Poincaré and log-Sobolev inequalities, for the matrix Φ -entropies. This framework is particularly useful for quantum information processing tasks that involve quantum systems carrying classical labels since a classical-quantum ensemble is a special type of a random matrix. As a result, matrix concentration inequalities developed in this work can help to provide a better illustration of the improvement caused by quantum communication or computation in the finite regime. As an example, we study how the Holevo quantity of a classical-quantum ensemble changes if the ensemble evolves according to a classical Markov kernel on its classical labels and a post-selection rule.

1.1. Our Results. The contribution of this paper is threefold.

- (1) First, we derive equivalent characterisations of the matrix Φ -entropies in Table 1. Notably, all known equivalent characterizations for the classical Φ -entropies can be generalised to their matrix correspondences.

	Classical Φ -Entropy Class (C1)	Matrix Φ -Entropy Class (C2)
(a)	Φ is affine or $\Phi'' > 0$ and $1/\Phi''$ is concave	Φ is affine or $D\Phi'$ is invertible and $(D\Phi')^{-1}$ is concave
(b)	convexity of $(u, v) \mapsto \Phi(u+v) - \Phi(u) - \Phi'(u)v$	convexity of $(\mathbf{u}, \mathbf{v}) \mapsto \text{Tr}[\Phi(\mathbf{u} + \mathbf{v}) - \Phi(\mathbf{u}) - D\Phi[\mathbf{u}](\mathbf{v})]$
(c)	convexity of $(u, v) \mapsto (\Phi'(u+v) - \Phi'(u))v$	convexity of $(\mathbf{u}, \mathbf{v}) \mapsto \text{Tr}[(D\Phi[\mathbf{u} + \mathbf{v}](\mathbf{v}) - D\Phi[\mathbf{u}](\mathbf{v})]$
(d)	convexity of $(u, v) \mapsto \Phi''(u)v^2$	convexity of $(\mathbf{u}, \mathbf{v}) \mapsto \text{Tr}[D^2\Phi[\mathbf{u}](\mathbf{v}, \mathbf{v})]$
(e)	Φ is affine or $\Phi'' > 0$ and $\Phi''' \Phi'' \geq 2\Phi''^2$	Equation (3.2)
(f)	convexity of $(u, v) \mapsto t\Phi(u) + (1-t)\Phi(v) - \Phi(tu + (1-t)v)$ for any $0 \leq t \leq 1$	convexity of $(\mathbf{u}, \mathbf{v}) \mapsto \text{Tr}[t\Phi(\mathbf{u}) + (1-t)\Phi(\mathbf{v}) - \Phi(t\mathbf{u} + (1-t)\mathbf{v})]$ for any $0 \leq t \leq 1$
(g)	$\mathbb{E}_1 H_\Phi(Z X_1) \geq H_\Phi(\mathbb{E}_1 Z)$	$\mathbb{E}_1 H_\Phi(\mathbf{Z} \mathbf{X}_1) \geq H_\Phi(\mathbb{E}_1 \mathbf{Z})$
(h)	$H_\Phi(Z)$ is a convex function of Z	$H_\Phi(\mathbf{Z})$ is a convex function of \mathbf{Z}
(i)	$H_\Phi(Z) = \sup_{T>0} \{\mathbb{E}[\Upsilon_1(T) \cdot Z + \Upsilon_2(T)]\}$	$H_\Phi(\mathbf{Z}) = \sup_{T>0} \{\overline{\text{tr}} \mathbb{E}[\Upsilon_1(T) \cdot \mathbf{Z} + \Upsilon_2(T)]\}$
(j)	$H_\Phi(Z) \leq \sum_{i=1}^n \mathbb{E} H_\Phi^{(i)}(Z)$	$H_\Phi(\mathbf{Z}) \leq \sum_{i=1}^n \mathbb{E} H_\Phi^{(i)}(\mathbf{Z})$

TABLE 1. Comparison between the equivalent characterizations of Φ -entropy functional class (C1) (Definition 3.1) and matrix Φ -entropy functional class (C2) (Definition 3.2)

We emphasize that additional characterizations of the Φ -entropies prove to be useful in many instances. The characterizations (b)-(d) in (C1) are explored by Chafaï [9] to derive several entropic inequalities for M/M/ ∞ queueing processes that are not diffusions. With the characterizations (b)-(d), the difficulty of lacking the diffusion property can be circumvented and replaced by convexity. The characterization (j) in (C1), also known as the subadditivity property, plays a crucial role in deriving powerful entropic inequalities for functions of a series of independent (not necessary identical) random variables, including Poincaré inequalities, Sobolev inequalities, logarithmic Sobolev inequalities, and Bousquet’s inequalities [6, 7]; while characterizations (g) and (i) are key steps to obtain (j) in (C1).

On the other hand, the characterization (b) in (C2)—the joint convexity of matrix Bréman divergence—is used to derive a sharp inequality for the quantum Tsallis entropy of a tripartite state. This is considered as a generalization of the strong subadditivity of the von Neumann entropy [13]. In this work, the characterization (j) in (C2) is shown to be crucial in deriving various entropic inequalities for matrix Φ -entropies, including matrix Poincaré inequalities and matrix Sobolev inequalities. Likewise, characterizations (g) and (i) are key steps to obtain (j) in (C2) [11].

- (2) After establishing equivalent characterizations of matrix Φ -entropies, we move on to derive matrix concentration inequalities, including matrix Poincaré inequalities, matrix Sobolev inequalities, and matrix logarithmic Sobolev inequalities. A fundamental tool used in the proofs is the subadditivity property of the matrix Φ -entropies.

- Poincaré inequality: We prove a Poincaré inequality for matrix-valued functions in Theorem 4.2 (see also Corollary 4.1), generalizing the classical Poincaré inequality [24, 25]:

$$(1.1) \quad \text{Var}(f(X)) \leq \mathbb{E} \left[\|\nabla f(X)\|^2 \right],$$

where $X \triangleq (X_1, \dots, X_n)$ denotes an independent random vector; each X_i taking values in the interval $[0, 1]$. Our proof, paralleling its classical counterpart, relies on the matrix-valued Efron-Stein inequality (Theorem 4.1). Both Theorem 4.2 and Corollary 4.1 recover the classical Poincaré inequality (1.1) when the matrix dimension $d = 1$.

We also derive various Poincaré inequalities for matrix-valued functions with additional assumptions such as pairwise commutation (Corollary 4.1) or Lipschitz functions (Corollary 4.2). Finally, we derive a matrix Gaussian Poincaré inequality for Gaussian Unitary Ensembles (Theorem 4.3).

- Φ -Sobolev inequality: We prove a restricted Φ -Sobolev inequality for matrix-valued functions defined on the Boolean hypercube in Theorem 4.5, from which we can also extend to a Φ -Sobolev inequality for Gaussian distributions (Theorem 4.6). Our Φ -Sobolev inequality is

defective (see Remark 4.5 for the discussions of *tight* and *defective* Φ -Sobolev inequalities), but again it recovers the classical Φ -Sobolev inequality when $d = 1$. Our proof builds upon a powerful matrix Bonami-Beckner inequality [18], from which the hypercontractivity inequality for matrix-valued functions on Boolean hypercubes can be obtained.

The matrix logarithmic Sobolev inequalities in Corollaries 4.3 and 4.4 follow immediately from Theorems 4.5 and 4.6.

- (3) Finally, we connect matrix Φ -entropies to quantum information theory. When $\Phi(x) = x \log x$ and the random matrix $\rho_X \equiv \{p(x), \rho_x\}_{x \in \mathcal{X}}$, where each $\rho_x \succeq 0$ and $\text{Tr } \rho_x = 1$, is a classical-quantum ensemble, $H_\Phi(\rho_X)$ is equal to the Holevo quantity $\chi(\{p, \rho\})$ (up to a constant dimensional factor for only technical purposes). If the ensemble $\rho_Y \equiv \{q(y), \sigma_y\}_{y \in \mathcal{Y}}$ is obtained by evolving ρ_X with a Markov kernel $K(y|x)$:

$$\begin{aligned} q(y) &= \sum_x p(x) K(y|x) \\ \sigma_y &= \sum_x \rho_x K^*(x|y) \end{aligned}$$

where $K^*(x|y)$ is the backward channel of K , then the Holevo quantity of $\chi(\{p, \rho\})$ is bounded from above by a constant c times the average Holevo quantity of the ensembles that come from post-selecting the original $\{p, \rho\}$ by the postselection rule K^* . Moreover, the constant c is related to the ratio of the Holevo quantities $\chi(\{p, \rho\})$ and $\chi(\{q, \sigma\})$ (see Proposition 5.1). This bears a stronger form of the classical strong data processing inequality [26, 27].

1.2. Prior work.

- (1) For the history of the equivalent characterizations in the class **(C1)**, we refer to an excellent textbook [5] and the papers [8, 9].

The original definition of the matrix Φ -entropy class; namely (a) in **(C2)**, is proposed by Chen and Tropp in 2014 [11]. In the same paper, they also establish the subadditivity property (j) through (i) and (g): (a) \Rightarrow (i) \Rightarrow (g) \Rightarrow (j). Shortly after, the equivalent relation between (a) and the joint convexity of the matrix Bréman divergence (b) is proved in [13]. The equivalent relation between (a) and (d) is almost immediately implied by the result in [12] (see the detailed discussion in the proof of Theorem 3.3).

- (2) Very few matrix concentration results have been established for general matrix-valued functions of independent random variables. To the best of our knowledge, the only gem in this area is a family of polynomial Efron-Stein inequalities for random matrices [28], where the theory of exchangeable pairs is used in the proof. In this work, we use the subadditivity property of the matrix Φ -entropies to derive an Efron-Stein inequality in Theorem 4.1, which is a special case of the result in [28] (for square functions). Note that in this special case, the constant in our theorem is better than that in [28].

We would also like to point out that the matrix Φ -entropies defined in the paper are different from the entropy functions in the non-commutative \mathbb{L}_p spaces in [16–23]. Currently, we do not know how to relate these two definitions. Hence, our matrix concentration inequalities in Section 4 are incomparable with those in the non-commutative \mathbb{L}_p spaces.

We organize the paper in the following way. Section 2 reviews Matrix Algebra necessary for the remaining of the paper. We show new characterizations of matrix Φ -entropies in Section 3. We then derive matrix concentration inequalities for matrix Φ -entropies in Section 4. We connect matrix Φ -entropies to quantum information theory in Section 5, and derive an upper bound on the Holevo quantity. Appendix A provides useful lemmas. We review the classical Bonami-Beckner inequality in Appendix B.

2. PRELIMINARIES

In this section we present the background information necessary for this paper. Basic notations are introduced in Section 2.1. We then review operator algebra with a focus on *Fréchet derivatives* and convexity properties of matrix-valued functions in Section 2.2 and 2.3, respectively.

2.1. Notation. Given a separable Hilbert space \mathcal{H} , denote by \mathbb{M} the Banach space of all linear operators on \mathcal{H} . The set \mathbb{M}^{sa} refers to the subspace of self-adjoint operators in \mathbb{M} . We denote by \mathbb{M}^+ (resp. \mathbb{M}^{++}) the set of positive semi-definite (resp. positive-definite) operators in \mathbb{M}^{sa} . If the dimension d of a Hilbert space \mathcal{H} needs special attention, then we highlight it in subscripts, e.g. \mathbb{M}_d denotes the Banach space of $d \times d$ complex matrices. For each interval $I \subset \mathbb{R}$, we define the set of self-adjoint operators whose eigenvalues lie in the interval to be:

$$\mathbb{M}^{\text{sa}}(I) \triangleq \{\mathbf{M} \in \mathbb{M}^{\text{sa}} : [\lambda_{\min}(\mathbf{M}), \lambda_{\max}(\mathbf{M})] \subset I\},$$

where $\lambda_{\min}(\mathbf{M})$ and $\lambda_{\max}(\mathbf{M})$ are the minimal and maximal eigenvalues of \mathbf{M} , respectively.

The trace function $\text{Tr} : \mathbb{M} \rightarrow \mathbb{C}$ is defined as

$$\text{Tr}[\mathbf{M}] \triangleq \sum_k e_k^* \mathbf{M} e_k \quad \text{for } \mathbf{M} \in \mathbb{M}$$

where $(e_k)_k$ is any orthonormal basis on \mathcal{H} . If we focus on finite dimensional Hilbert spaces, then the trace function acting on \mathbf{M} is equal to the summation of its eigenvalues. In this paper, we introduce the normalised trace function $\overline{\text{tr}}$ for every matrix $\mathbf{M} \in \mathbb{M}_d$ as

$$\overline{\text{tr}}[\mathbf{M}] \triangleq \frac{1}{d} \text{Tr}[\mathbf{M}].$$

The normalised trace function enjoys a convexity property (see Lemma 2.1), which will be convenient for later derivations in this paper.

For $p \in [1, \infty)$, the Schatten p -norm of an operator $\mathbf{M} \in \mathbb{M}$ is denoted as

$$(2.1) \quad \|\mathbf{M}\|_p \triangleq \left(\sum_i |\lambda_i(\mathbf{M})|^p \right)^{1/p},$$

where $\{\lambda_i(\mathbf{M})\}$ are the singular values of \mathbf{M} . We also define the supremum norm of a (finite or infinite) matrix $\mathbf{M} \in \mathbb{M}$ as

$$\|\mathbf{M}\|_{\text{sup}} \triangleq \sup_{i,j} |M_{ij}|.$$

Define \mathbb{S}^n to be the set of all mutually commuting n -tuple self-adjoint operators; namely, if $\mathbf{X} = (\mathbf{X}_1, \dots, \mathbf{X}_n) \in \mathbb{S}^n$, then $[\mathbf{X}_i, \mathbf{X}_j] = \mathbf{0}$ for $i \neq j \in [n]$. We denote by \mathbb{S}_d^n the set of mutually commuting n -tuple $d \times d$ Hermitian matrices.

For $\mathbf{A}, \mathbf{B} \in \mathbb{M}^{\text{sa}}$, $\mathbf{A} \succeq \mathbf{B}$ means that $\mathbf{A} - \mathbf{B}$ is positive semi-definite. Similarly, $\mathbf{A} \succ \mathbf{B}$ means $\mathbf{A} - \mathbf{B}$ is positive-definite.

Throughout this paper, italic capital letters (e.g. \mathbf{X}) are used to denote operators, and non-italic ones (e.g. \mathbf{X}) are used to denote a collection of, say n , operators.

2.2. Matrix Calculus. In this section, we only provide sufficient information for the matrix calculus. For a general treatment of this topic, interested readers can refer to [29, Section 2.1], [30, Chapter 17], [31, Section X.4], [32, Section 5.3], and [33, Chapter 3].

Let \mathcal{U}, \mathcal{W} be real Banach spaces. The *Fréchet derivative* of a function $\mathcal{L} : \mathcal{U} \rightarrow \mathcal{W}$ at a point $\mathbf{X} \in \mathcal{U}$, if it exists¹, is a unique linear mapping $\text{D}\mathcal{L}[\mathbf{X}] : \mathcal{U} \rightarrow \mathcal{W}$ such that

$$\frac{\|\mathcal{L}(\mathbf{X} + \mathbf{E}) - \mathcal{L}(\mathbf{X}) - \text{D}\mathcal{L}[\mathbf{X}](\mathbf{E})\|_{\mathcal{W}}}{\|\mathbf{E}\|_{\mathcal{U}}} \rightarrow 0 \quad \text{as } \mathbf{E} \in \mathcal{U} \text{ and } \|\mathbf{E}\|_{\mathcal{U}} \rightarrow \mathbf{0},$$

or, equivalently,

$$\|\mathcal{L}(\mathbf{X} + \mathbf{E}) - \mathcal{L}(\mathbf{X}) - \text{D}\mathcal{L}[\mathbf{X}](\mathbf{E})\|_{\mathcal{W}} = o(\|\mathbf{E}\|_{\mathcal{U}}),$$

where $\|\cdot\|_{\mathcal{U}(\mathcal{W})}$ is a norm in \mathcal{U} (resp. \mathcal{W}). The notation $\text{D}\mathcal{L}[\mathbf{X}](\mathbf{E})$ then is interpreted as “the Fréchet derivative of \mathcal{L} at \mathbf{X} in the direction \mathbf{E} ”. Furthermore, the Fréchet derivative implies the Gâteaux derivative such that the differentiation of $\mathcal{L}(\mathbf{X} + t\mathbf{E})$ with respect to the real variable t is

$$\frac{\mathcal{L}(\mathbf{X} + t\mathbf{E}) - \mathcal{L}(\mathbf{X})}{t} \rightarrow \text{D}\mathcal{L}[\mathbf{X}](\mathbf{E}) \quad \text{as } t \rightarrow 0.$$

¹We assume the functions considered in the paper are Fréchet differentiable. The readers can refer to, e.g. [34, 35], for conditions for when a function is Fréchet differentiable.

For example, if the operator-valued function is the inversion $\mathcal{L}(\mathbf{X}) = \mathbf{X}^{-1}$ for each invertible matrix \mathbf{X} , then (see e.g. [31, Example X.4.2])

$$(2.2) \quad \mathrm{D}\mathcal{L}[\mathbf{X}](\mathbf{Y}) = -\mathbf{X}^{-1}\mathbf{Y}\mathbf{X}^{-1} \quad \text{for all } \mathbf{Y} \in \mathbb{M}.$$

The Fréchet derivative also satisfies several properties similar to conventional derivatives of real-valued functions (see e.g. [33, Theorem 3.4]):

Proposition 2.1 (Properties of Fréchet Derivatives). *Let \mathcal{U}, \mathcal{V} and \mathcal{W} be real Banach spaces.*

1. (Sum Rule) *If $\mathcal{L}_1 : \mathcal{U} \rightarrow \mathcal{W}$ and $\mathcal{L}_2 : \mathcal{U} \rightarrow \mathcal{W}$ are Fréchet differentiable at $\mathbf{A} \in \mathcal{U}$, then so is $\mathcal{L} = \alpha\mathcal{L}_1 + \beta\mathcal{L}_2$ and $\mathrm{D}\mathcal{L}[\mathbf{A}](\mathbf{E}) = \alpha \cdot \mathrm{D}\mathcal{L}_1[\mathbf{A}](\mathbf{E}) + \beta \cdot \mathrm{D}\mathcal{L}_2[\mathbf{A}](\mathbf{E})$.*
2. (Product Rule) *If $\mathcal{L}_1 : \mathcal{U} \rightarrow \mathcal{W}$ and $\mathcal{L}_2 : \mathcal{U} \rightarrow \mathcal{W}$ are Fréchet differentiable at $\mathbf{A} \in \mathcal{U}$ and assume the multiplication is well-defined in \mathcal{W} , then so is $\mathcal{L} = \mathcal{L}_1 \cdot \mathcal{L}_2$ and $\mathrm{D}\mathcal{L}[\mathbf{A}](\mathbf{E}) = \mathrm{D}\mathcal{L}_1[\mathbf{A}](\mathbf{E}) \cdot \mathcal{L}_2(\mathbf{A}) + \mathcal{L}_1(\mathbf{A}) \cdot \mathrm{D}\mathcal{L}_2[\mathbf{A}](\mathbf{E})$.*
3. (Chain Rule) *Let $\mathcal{L}_1 : \mathcal{U} \rightarrow \mathcal{V}$ and $\mathcal{L}_2 : \mathcal{V} \rightarrow \mathcal{W}$ be Fréchet differentiable at $\mathbf{A} \in \mathcal{U}$ and $\mathcal{L}_1(\mathbf{A})$ respectively, and let $\mathcal{L} = \mathcal{L}_2 \circ \mathcal{L}_1$ (i.e. $\mathcal{L}(\mathbf{A}) = \mathcal{L}_2(\mathcal{L}_1(\mathbf{A}))$). Then \mathcal{L} is Fréchet differentiable at \mathbf{A} and $\mathrm{D}\mathcal{L}[\mathbf{A}](\mathbf{E}) = \mathrm{D}\mathcal{L}_2[\mathcal{L}_1(\mathbf{A})](\mathrm{D}\mathcal{L}_1[\mathbf{A}](\mathbf{E}))$.*

Similarly, the m -th Fréchet derivative $\mathrm{D}^m\mathcal{L}[\mathbf{X}]$ is a unique multi-linear map from $\mathcal{U}^m \triangleq \mathcal{U} \times \cdots \times \mathcal{U}$ (m times) to \mathcal{W} that satisfies

$$\begin{aligned} & \|\mathrm{D}^{m-1}\mathcal{L}[\mathbf{X} + \mathbf{E}_m](\mathbf{E}_1, \dots, \mathbf{E}_{m-1}) - \mathrm{D}^{m-1}\mathcal{L}[\mathbf{X}](\mathbf{E}_1, \dots, \mathbf{E}_{m-1}) \\ & \quad - \mathrm{D}^m\mathcal{L}[\mathbf{X}](\mathbf{E}_1, \dots, \mathbf{E}_m)\|_{\mathcal{W}} = o(\|\mathbf{E}_m\|_{\mathcal{U}}) \end{aligned}$$

for each $\mathbf{E}_i \in \mathcal{U}, i = 1, \dots, m$. If $\mathrm{D}^m\mathcal{L}[\mathbf{X}]$ is continuous at \mathbf{X} , then the m -th Fréchet derivative can be expressed as a mixed partial derivative [36, Section 9] (see also [37, Theorem 2.3.1]).

$$\mathrm{D}^m\mathcal{L}[\mathbf{X}](\mathbf{E}_1, \dots, \mathbf{E}_m) = \left. \frac{\partial}{\partial s_1} \cdots \frac{\partial}{\partial s_m} \right|_{s_1=\dots=s_m=0} \mathcal{L}(\mathbf{X} + s_1\mathbf{E}_1 + \cdots + s_m\mathbf{E}_m).$$

We can observe, from the above equation, that the m -th Fréchet derivative is symmetric about all \mathbf{E}_i ; see [38, Theorem 8], [31, p. 313], and [39, Theorem 4.3.4]. We refer to Refs. [40, Section 8.12], [30, Chapter 17], [39, Section 4.3], and [41] for further information about higher order Fréchet derivatives.

The following proposition relates the second order Fréchet derivative with the convexity of a matrix-valued function, i.e. $\mathcal{L}(t\mathbf{A}) + \mathcal{L}((1-t)\mathbf{B}) \preceq \mathcal{L}(t\mathbf{A} + (1-t)\mathbf{B})$ for all $0 \leq t \leq 1$.

Proposition 2.2 (Convexity of twice Fréchet differentiable matrix functions [42, Proposition 2.2]). *Let U be an open convex subset of a real Banach space \mathcal{U} , and \mathcal{W} is also a real Banach space. Then a twice Fréchet differentiable function $\mathcal{L} : U \rightarrow \mathcal{W}$ is convex if and only if $\mathrm{D}^2\mathcal{L}(\mathbf{X})(\mathbf{h}, \mathbf{h}) \succeq \mathbf{0}$ for each $\mathbf{X} \in U$ and $\mathbf{h} \in \mathcal{U}$.*

The *partial Fréchet derivative* of multivariate functions can be defined as follows [32, Section 5.3]. Let \mathcal{U}, \mathcal{V} and \mathcal{W} be real Banach spaces, $\mathcal{L} : \mathcal{U} \times \mathcal{V} \rightarrow \mathcal{W}$. For a fixed $\mathbf{v}_0 \in \mathcal{V}$, $\mathcal{L}(\mathbf{u}, \mathbf{v}_0)$ is a function of \mathbf{u} whose derivative at \mathbf{u}_0 , if it exists, is called the partial Fréchet derivative of \mathcal{L} with respect to \mathbf{u} , and is denoted by $\mathrm{D}_{\mathbf{u}}\mathcal{L}[\mathbf{u}_0, \mathbf{v}_0]$. The partial Fréchet derivative $\mathrm{D}_{\mathbf{v}}\mathcal{L}[\mathbf{u}_0, \mathbf{v}_0]$ is defined similarly.

The Fréchet derivative and the partial Fréchet derivative can be related as follows.

Proposition 2.3 (Partial Fréchet derivative [32, Proposition 5.3.15]). *If $\mathcal{L} : \mathcal{U} \times \mathcal{V} \rightarrow \mathcal{W}$ is Fréchet differentiable at $(\mathbf{X}, \mathbf{Y}) \in \mathcal{U} \times \mathcal{V}$, then the partial Fréchet derivatives $\mathrm{D}_{\mathbf{X}}\mathcal{L}[\mathbf{X}, \mathbf{Y}]$ and $\mathrm{D}_{\mathbf{Y}}\mathcal{L}[\mathbf{X}, \mathbf{Y}]$ exist, and*

$$\mathrm{D}\mathcal{L}[\mathbf{X}, \mathbf{Y}](\mathbf{h}, \mathbf{k}) = \mathrm{D}_{\mathbf{X}}\mathcal{L}[\mathbf{X}, \mathbf{Y}](\mathbf{h}) + \mathrm{D}_{\mathbf{Y}}\mathcal{L}[\mathbf{X}, \mathbf{Y}](\mathbf{k}).$$

Now let $\mathcal{L} : \mathcal{U}^n \rightarrow \mathcal{W}$ and assume it is a holomorphic function (i.e. Fréchet differential in a neighborhood of every point in its domain), then the *Taylor expansion* $\mathcal{L}(\mathbf{X} + \mathbf{E})$ at $\mathbf{X} \triangleq (\mathbf{X}_1, \dots, \mathbf{X}_n) \in \mathcal{U}^n$ can be

expressed as

$$\begin{aligned}
\mathcal{L}(\mathbf{X} + \mathbf{E}) &= \mathcal{L}(\mathbf{X}) + \sum_{k=1}^{\infty} \frac{1}{k!} \mathbf{D}^k \mathcal{L}[\mathbf{X}] (\underbrace{\mathbf{E}, \dots, \mathbf{E}}_k) \\
(2.3) \quad &= \mathcal{L}(\mathbf{X}) + \sum_{j=1}^n \mathbf{D}_{\mathbf{X}_j} \mathcal{L}[\mathbf{X}] (\mathbf{E}_j) + \frac{1}{2!} \sum_{j=1}^n \sum_{k=1}^n \mathbf{D}_{\mathbf{X}_j \mathbf{X}_k}^2 (\mathbf{E}_j, \mathbf{E}_k) + \text{Remaining terms.}
\end{aligned}$$

For any map $\mathcal{L} : \mathcal{U} \rightarrow \mathcal{W}$ and an operator $\mathbf{X} \in \mathcal{U}$, we define the induced norm of the Fréchet derivative $\mathbf{D}\mathcal{L}[\mathbf{X}]$ as

$$(2.4) \quad \|\mathbf{D}\mathcal{L}[\mathbf{X}]\| \triangleq \sup_{\mathbf{E} \neq \mathbf{0}} \frac{\|\mathbf{D}\mathcal{L}[\mathbf{X}](\mathbf{E})\|}{\|\mathbf{E}\|},$$

where the norm can be any consistent norm (e.g. $\|\mathbf{D}\mathcal{L}[\mathbf{X}]\|_2 = \sup_{\mathbf{E} \neq \mathbf{0}} \|\mathbf{D}\mathcal{L}[\mathbf{X}](\mathbf{E})\|_2 / \|\mathbf{E}\|_2$).

The norm of the Fréchet derivative is closely related to the condition numbers, which measure the sensitivity of an operator-valued function to perturbations in the variables. Hence, the *absolute condition number* is defined by

$$(2.5) \quad \text{cond}_{\text{abs}}(\mathcal{L}, \mathbf{X}) \triangleq \lim_{\epsilon \rightarrow 0} \sup_{\|\mathbf{E}\| \leq \epsilon} \frac{\|\mathcal{L}(\mathbf{X} + \mathbf{E}) - \mathcal{L}(\mathbf{X})\|}{\epsilon}.$$

Then the norm of the Fréchet derivative can be expressed by the absolute condition number [43]

$$\text{cond}_{\text{abs}}(\mathcal{L}, \mathbf{X}) = \|\mathbf{D}\mathcal{L}[\mathbf{X}]\|.$$

We note that there are several algorithms and software packages that can compute the absolute condition number; see [33, Section 3], [44] and references therein.

2.3. Standard Matrix Functions. In this section, we restrict our considerations to the *standard matrix functions*. Coupled with the techniques of matrix calculus described above, standard matrix functions enjoy additional properties which are useful throughout this work.

For each self-adjoint and bounded operator $\mathbf{A} \in \mathbb{M}^{\text{sa}}$ with the spectrum $\sigma(\mathbf{A})$ and the spectral measure \mathbf{E} , the *spectral decomposition* is given as

$$(2.6) \quad \mathbf{A} = \int_{\lambda \in \sigma(\mathbf{A})} \lambda \, \mathbf{d}\mathbf{E}(\lambda).$$

Hence, each scalar function can be extended to a standard matrix function as follows.

Definition 2.1 (Standard Matrix Function). Let $f : I \rightarrow \mathbb{R}$ be a real-valued function on an interval I of the real line. Suppose that $\mathbf{A} \in \mathbb{M}^{\text{sa}}(I)$ has the spectral decomposition (2.6). Then

$$f(\mathbf{A}) \triangleq \int_{\lambda \in \sigma(\mathbf{A})} f(\lambda) \, \mathbf{d}\mathbf{E}(\lambda).$$

From this equation, it is clear that $\sigma(f(\mathbf{A})) = f(\sigma(\mathbf{A}))$, which is called the *spectral mapping theorem*.

Note that we use lowercase Roman and Greek letters to denote standard matrix functions, while calligraphic capital letters \mathcal{L} refer to general operator-valued functions that are not necessarily standard.

The spectral mapping theorem of standard matrix functions immediately yields the following convexity property of the normalised trace function.

Lemma 2.1 (Convexity Lemma for Normalised Trace Functions). *For every convex function $f : I \rightarrow \mathbb{R}$ and every matrix $\mathbf{A} \in \mathbb{M}_d^{\text{sa}}(I)$, we have the following relation*

$$\overline{\text{tr}} f(\mathbf{A}) \geq f(\overline{\text{tr}} \mathbf{A}).$$

Proof. The convexity lemma follows from the fact that the normalised trace is a convex combination of the eigenvalues. More specifically,

$$\begin{aligned}\overline{\text{tr}} f(\mathbf{A}) &= \frac{1}{d} \sum_{i=1}^d \lambda_i(f(\mathbf{A})) = \frac{1}{d} \sum_{i=1}^d f(\lambda_i(\mathbf{A})) \\ &\geq f\left(\frac{1}{d} \sum_{i=1}^d \lambda_i(\mathbf{A})\right) = f(\overline{\text{tr}} \mathbf{A}),\end{aligned}$$

where in the second identity we use the spectral mapping theorem and the third relation is due to the convexity of f . \square

A function $f : I \rightarrow \mathbb{R}$ is called *operator convex* if for each $\mathbf{A}, \mathbf{B} \in \mathbb{M}^{\text{sa}}(I)$ and $0 \leq t \leq 1$,

$$f(t\mathbf{A}) + f((1-t)\mathbf{B}) \preceq f(t\mathbf{A} + (1-t)\mathbf{B}).$$

Similarly, a function $f : I \rightarrow \mathbb{R}$ is called *operator monotone* if for each $\mathbf{A}, \mathbf{B} \in \mathbb{M}^{\text{sa}}(I)$,

$$\mathbf{A} \preceq \mathbf{B} \Rightarrow f(\mathbf{A}) \preceq f(\mathbf{B}).$$

It is remarkable that not all convex (resp. monotone) functions are operator convex (resp. monotone). For example, the exponential function is not operator convex nor operator monotone on $[0, \infty)$; the power functions that are operator convex are $f(x) = x^p$ for $p \in [-1, 0] \cup [1, 2]$ and $f(x) = -x^p$ for $p \in [0, 1]$. However, the trace function on \mathbb{M}^{sa} given by $\mathbf{A} \rightarrow \text{Tr}[f(\mathbf{A})]$ preserves the convexity or monotonicity.

Proposition 2.4 (Convexity and Monotonicity for Trace Functions [45, Section 2.2]). *Consider a real-valued function $f : I \rightarrow \mathbb{R}$. If f is convex (resp. monotone) on $U \subseteq I$, then the function $\mathbf{A} \rightarrow \text{Tr}[f(\mathbf{A})]$ is convex (resp. monotone) on $\mathbb{M}^{\text{sa}}(U)$.*

We refer the readers to Refs. [37] and [46] for general expositions to operator convex and monotone functions.

If the scalar function is continuously differentiable, then it is convenient to introduce the following two properties for the trace function of Fréchet derivatives.

Proposition 2.5 ([46, Theorem 3.23]). *Let $\mathbf{A}, \mathbf{X} \in \mathbb{M}^{\text{sa}}$ and $t \in \mathbb{R}$. Assume $f : I \rightarrow \mathbb{R}$ is a continuously differentiable function defined on interval I and assume that the eigenvalues of $\mathbf{A} + t\mathbf{X} \subset I$. Then*

$$\left. \frac{d}{dt} \text{Tr} f(\mathbf{A} + t\mathbf{X}) \right|_{t=t_0} = \text{Tr}[\mathbf{X} f'(\mathbf{A} + t_0\mathbf{X})].$$

Lemma 2.2. *Let $\mathbf{A}, \mathbf{X}, \mathbf{Y} \in \mathbb{M}^{\text{sa}}$ and $t \in \mathbb{R}$. Assume $f : I \rightarrow \mathbb{R}$ is a continuously differentiable function defined on interval I , and assume that the eigenvalues of $\mathbf{A} + t\mathbf{X} \subset I$. Then*

$$\begin{aligned}\text{Tr}(\mathbf{D}^2 f[\mathbf{A}](\mathbf{X}, \mathbf{Y})) &= \langle \mathbf{X}, \mathbf{D}f'[\mathbf{A}](\mathbf{Y}) \rangle \\ &= \langle \mathbf{Y}, \mathbf{D}f'[\mathbf{A}](\mathbf{X}) \rangle.\end{aligned}$$

Proof. By applying Fubini's theorem, we can interchange the order of trace and Fréchet derivative to obtain

$$\begin{aligned}\text{Tr}(\mathbf{D}^2 f[\mathbf{A}](\mathbf{X}, \mathbf{Y})) &= \text{Tr} \left[\left. \frac{\partial^2}{\partial t \partial s} f(\mathbf{A} + s\mathbf{X} + t\mathbf{Y}) \right|_{t=0, s=0} \right] \\ &= \frac{\partial}{\partial t} \left[\left. \frac{\partial}{\partial s} \text{Tr} f(\mathbf{A} + s\mathbf{X} + t\mathbf{Y}) \right|_{s=0} \right]_{t=0} \\ &= \frac{\partial}{\partial t} \text{Tr}[\mathbf{X} f'(\mathbf{A} + t\mathbf{Y})] \Big|_{t=0} \\ &= \text{Tr}[\mathbf{X} \cdot \mathbf{D}f'[\mathbf{A}](\mathbf{Y})] \\ &= \langle \mathbf{X}, \mathbf{D}f'[\mathbf{A}](\mathbf{Y}) \rangle,\end{aligned}$$

where the third identity follows from Proposition 2.5.

Since $D^2 f[\mathbf{A}]$ is symmetric in the sense that $D^2 f[\mathbf{A}](\mathbf{X}, \mathbf{Y}) = D^2 f[\mathbf{A}](\mathbf{Y}, \mathbf{X})$, the second equation follows similarly. \square

It is useful to express the Fréchet differentiation as the *divided differences*. Let a_1, a_2, \dots be distinct real points on $I \subseteq \mathbb{R}$. Then we define the zero and first order divided differences as

$$f^{[0]}(a_1) \triangleq f(a_1), \quad f^{[1]}(a_1, a_2) \triangleq \frac{f(a_1) - f(a_2)}{a_1 - a_2},$$

and n -th order divided difference

$$f^{[n]}(a_1, \dots, a_{n+1}) \triangleq \frac{f^{[n-1]}(a_1, a_2, \dots, a_n) - f^{[n-1]}(a_2, a_3, \dots, a_{n+1})}{a_1 - a_{n+1}}.$$

Therefore, the following formula gives the explicit form for the Fréchet derivative of a standard matrix function.

Proposition 2.6 (Daleckiĭ and Kreĭn Formula [33, Theorem 3.11]). *When f is first-order differentiable on $I \subseteq \mathbb{R}$ and $\mathbf{A} = \text{diag}(a_1, \dots, a_d)$ is diagonal in $\mathbb{M}_d^{\text{sa}}(I)$, then the first-order Fréchet derivative $Df[\mathbf{A}]$ at \mathbf{A} can be written as*

$$Df[\mathbf{A}](\mathbf{X}) = \left[f^{[1]}(a_i, a_j) \right]_{i,j=1}^d \odot \mathbf{X},$$

where \odot denotes the Schur product. Moreover, as f is second-order differentiable on I , the corresponding second-order Fréchet derivative is

$$D^2 f[\mathbf{A}](\mathbf{X}, \mathbf{Y}) = \left[\sum_{k=1}^n f^{[2]}(a_i, a_k, a_j) (X_{ik} Y_{kj} + Y_{ik} X_{kj}) \right]_{i,j=1}^n.$$

The standard matrix function can be extended into the multivariate case by considering n -tuples commuting self-adjoint operators.

Definition 2.2 (Multivariate Matrix Function). Let $\mathbf{X} = (\mathbf{X}_1, \dots, \mathbf{X}_n) \in \mathbb{S}^n(I)$ be an n -tuples commuting self-adjoint operators with the spectral decomposition $\mathbf{X}_i = \int_{\lambda \in I_i} \lambda d\mathbf{E}_i(\lambda)$. Since \mathbf{X}_i 's commute, define the product spectral measure on $\underline{I} \triangleq I_1 \times \dots \times I_n$ as $\mathbf{E}(\lambda_1, \dots, \lambda_n) \triangleq \mathbf{E}(\lambda_1) \cdots \mathbf{E}(\lambda_n)$. Then,

$$f(\mathbf{X}) \triangleq \int_{(\lambda_1, \dots, \lambda_n) \in \underline{I}} f(\lambda_1, \dots, \lambda_n) d\mathbf{E}(\lambda_1, \dots, \lambda_n).$$

For each $i = 1, \dots, n$, the (first-order) divided difference of multivariate matrix function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is defined by the rule

$$\varphi_i^f(\bar{x}, \bar{y}) = \frac{(f(\bar{x} - \bar{y}))(x_i - y_i)}{\|\bar{x} - \bar{y}\|_2^2} \text{ for } \bar{x} \neq \bar{y} \quad \text{and} \quad \varphi_k^f(\bar{x}, \bar{x}) = \frac{\partial f}{\partial x_i}(\bar{x}),$$

where $\bar{x} \triangleq (x_1, \dots, x_n) \in \mathbb{R}^n$. We will just denote it by φ_i if no confusion is possible.

Via the introduced divided difference function, Proposition 2.6 can be extended to multivariate matrix functions. More precisely, for each $i = 1, \dots, n$, the partial Fréchet derivative can be expressed as

$$(2.7) \quad D_{\mathbf{X}_i} f[\mathbf{X}](\mathbf{E}) = [\varphi_i(\bar{\lambda}_k, \bar{\lambda}_l)]_{kl} \odot \mathbf{E}, \quad \forall \mathbf{X} \in \mathbb{S}^n \text{ and } \mathbf{E} \in \mathbb{M}^{\text{sa}},$$

where the $\{\mathbf{X}_i\}_{i=1}^n$ are simultaneously diagonalised with λ_{ik} being the k -th eigenvalue of \mathbf{X}_i and $\bar{\lambda}_k \triangleq (\lambda_{1k}, \dots, \lambda_{nk})$.

Remark 2.1. To the best of our knowledge, there are four types of definitions for the multivariate standard matrix functions. Our treatment of multivariate standard matrix functions on n -tuples commuting self-adjoint operators originates from Lieb and Pedersen [47, 48] (see also [49, 50] for applications). Hansen *et al.* also introduced an alternate approach by viewing $f(\mathbf{X})$ as an operator in $\mathbb{M}^{\text{sa}} \otimes \dots \otimes \mathbb{M}^{\text{sa}}$ [42, 51–54]. Kressner [55] proposed a method by considering $f(\mathbf{X})$ as a super-operator on $\mathbb{M}^{\text{sa}} \otimes \dots \otimes \mathbb{M}^{\text{sa}}$. Very recently, there was a non-commutative generalisation of the multivariate standard matrix; see [56–59]. However, the results are still limited. \diamond

3. NEW CHARACTERIZATIONS OF MATRIX Φ -ENTROPY FUNCTIONALS

We first introduce classical Φ -entropies and its subadditivity property in Section 3.1. The readers may refer to [8, 9, 25, 60, 61] and [5, Chapter 14] for more comprehensive discussions. Then, we move on to introduce matrix Φ -entropies in Section 3.2, and present the main result (Theorem 3.3) of this section; namely, new characterizations of the matrix Φ -entropies.

3.1. Classical Φ -Entropies. Let $(\mathbf{C1})$ denote the class of functions $\Phi : [0, \infty) \rightarrow \mathbb{R}$ that are continuous, convex on $[0, \infty)$, twice differentiable on $(0, \infty)$, and either Φ is affine or Φ'' is strictly positive and $1/\Phi''$ is concave.

Definition 3.1 (Classical Φ -Entropies). Consider $\Phi \in (\mathbf{C1})$. For every non-negative integrable random variable Z so that $\mathbb{E}|Z| < \infty$ and $\mathbb{E}|\Phi(Z)| < \infty$, the classical Φ -entropy $H_\Phi(Z)$ is defined as

$$H_\Phi(Z) = \mathbb{E}\Phi(Z) - \Phi(\mathbb{E}Z).$$

In particular, we are interested in $Z = f(X_1, \dots, X_n)$, where X_1, \dots, X_n are independent random variables, and $f \geq 0$ is a measurable function.

We say $H_\Phi(Z)$ is *subadditive* [25] if

$$H_\Phi(Z) \leq \sum_{i=1}^n \mathbb{E}H_\Phi^{(i)}(Z),$$

where $H_\Phi^{(i)}(Z) = \mathbb{E}_i\Phi(Z) - \Phi(\mathbb{E}_iZ)$ is the conditional Φ -entropy, and \mathbb{E}_i denotes conditional expectation conditioned on the $n-1$ random variables $X_{-i} \triangleq (X_1, \dots, X_{i-1}, X_{i+1}, \dots, X_n)$. Sometimes we also denote $H_\Phi^{(i)}(Z)$ by $H_\Phi(Z|X_{-i})$.

It is a well-known result that, for any function $\Phi \in (\mathbf{C1})$, $H_\Phi(Z)$ is subadditive [61, Corollary 3] (see also [60, Section 3]).

The following theorem establishes equivalent characterizations of classical Φ -entropies.

Theorem 3.1 ([9, Theorem 4.4]). *The following statements are equivalent.*

- (a) $\Phi \in (\mathbf{C1})$: Φ is affine or $\Phi'' > 0$ and $1/\Phi''$ is concave;
- (b) Brègman divergence $(u, v) \mapsto \Phi(u+v) - \Phi(u) - \Phi'(u)v$ is convex;
- (c) $(u, v) \mapsto (\Phi'(u+v) - \Phi'(u))v$ is convex;
- (d) $(u, v) \mapsto \Phi''(u)v^2$ is convex;
- (e) Φ is affine or $\Phi'' > 0$ and $\Phi''' \Phi'' \geq 2\Phi''^2$;
- (f) $(u, v) \mapsto t\Phi(u) + (1-t)\Phi(v) - \Phi(tu + (1-t)v)$ is convex for any $0 \leq t \leq 1$;
- (g) $\mathbb{E}_1 H_\Phi(Z|X_1) \geq H_\Phi(\mathbb{E}_1 Z)$;
- (h) $\{H_\Phi(Z)\}_{\Phi \in (\mathbf{C1})}$ forms a convex set;
- (i) $H_\Phi(Z) = \sup_{T>0} (\mathbb{E}[(\Phi'(T) - \Phi'(\mathbb{E}T))(Z - T)] + H_\Phi(T))$;
- (j) $H_\Phi(Z) \leq \sum_{i=1}^n \mathbb{E}H_\Phi^{(i)}(Z)$.

3.2. Matrix Φ -entropies. Chen and Tropp introduce the class of matrix Φ -entropies, and prove its subadditivity in 2014 [11]. In this section, we will show that all equivalent characterizations of classical Φ -entropies in Theorem 3.1 have a one-to-one correspondence for the class of matrix Φ -entropies.

Let d be a natural number. The class Φ_d contains each function $\Phi : (0, \infty) \rightarrow \mathbb{R}$ that is either affine or satisfies the following three conditions:

- (1) Φ is convex and continuous at zero.
- (2) Φ is twice continuously differentiable.
- (3) Define $\Psi(t) = \Phi'(t)$ for $t > 0$. The Fréchet derivative $D\Psi$ of the standard matrix function $\Psi : \mathbb{M}_d^{++} \rightarrow \mathbb{M}_d^{\text{sa}}$ is an invertible linear map on \mathbb{M}_d^{++} , and the map $\mathbf{A} \mapsto (D\Psi[\mathbf{A}])^{-1}$ is concave with respect to the Löwner partial ordering on positive definite matrices.

Define $(\mathbf{C2}) \triangleq \Phi_\infty \equiv \bigcap_{d=1}^\infty \Phi_d$.

Definition 3.2 (Matrix Φ -Entropies [11]). Let $\Phi \in \Phi_\infty$. Consider a random matrix $\mathbf{Z} \in \mathbb{M}_d^+$ with $\mathbb{E}\|\mathbf{Z}\|_\infty < \infty$ and $\mathbb{E}\|\Phi(\mathbf{Z})\|_\infty < \infty$. The matrix Φ -entropy $H_\Phi(\mathbf{Z})$ is defined as

$$H_\Phi(\mathbf{Z}) \triangleq \overline{\text{tr}}[\mathbb{E}\Phi(\mathbf{Z}) - \Phi(\mathbb{E}\mathbf{Z})].$$

The corresponding conditional matrix Φ -entropy can be defined under the σ -algebra.

Theorem 3.2 (Subadditivity of Matrix Φ -Entropies [11]). Let $\Phi \in (\mathcal{C}2)$, and assume \mathbf{Z} is a measurable function of $(\mathbf{X}_1, \dots, \mathbf{X}_n)$.

$$(3.1) \quad H_\Phi(\mathbf{Z}) \leq \sum_{i=1}^n \mathbb{E}[H_\Phi^{(i)}(\mathbf{Z})],$$

where $H_\Phi^{(i)}(\mathbf{Z}) = \mathbb{E}_i\Phi(\mathbf{Z}) - \Phi(\mathbb{E}_i\mathbf{Z})$ is the conditional entropy, and \mathbb{E}_i denotes conditional expectation conditioned on the $n-1$ random matrices $\mathbf{X}_{-i} \triangleq (\mathbf{X}_1, \dots, \mathbf{X}_{i-1}, \mathbf{X}_{i+1}, \dots, \mathbf{X}_n)$.

The following theorem is the main result of the section. It establishes that all the equivalent conditions in Theorem 3.1 also hold for the class of matrix Φ -entropies.

Theorem 3.3. The following statements are equivalent.

- (a) $\Phi \in (\mathcal{C}2)$: Φ is affine or $\mathcal{D}\Psi$ is invertible and $\mathbf{A} \mapsto (\mathcal{D}\Psi[\mathbf{A}])^{-1}$ is operator concave;
- (b) Matrix Brègman divergence: $(\mathbf{A}, \mathbf{B}) \mapsto \text{Tr}[\Phi(\mathbf{A} + \mathbf{B}) - \Phi(\mathbf{A}) - \mathcal{D}\Phi[\mathbf{A}](\mathbf{B})]$ is convex;
- (c) $(\mathbf{A}, \mathbf{B}) \mapsto \text{Tr}[\mathcal{D}\Phi[\mathbf{A} + \mathbf{B}](\mathbf{B}) - \mathcal{D}\Phi[\mathbf{A}](\mathbf{B})]$ is convex;
- (d) $(\mathbf{A}, \mathbf{B}) \mapsto \text{Tr}[\mathcal{D}^2\Phi[\mathbf{A}](\mathbf{B}, \mathbf{B})]$ is convex;
- (e) Φ is affine or $\Phi'' > 0$ and

$$(3.2) \quad \begin{aligned} & \text{Tr} \left[\mathbf{h} \cdot (\mathcal{D}\Psi[\mathbf{A}])^{-1} \circ \mathcal{D}^3\Psi[\mathbf{A}] \left(\mathbf{k}, \mathbf{k}, (\mathcal{D}\Psi[\mathbf{A}])^{-1}(\mathbf{h}) \right) \right] \\ & \geq 2 \text{Tr} \left[\mathbf{h} \cdot (\mathcal{D}\Psi[\mathbf{A}])^{-1} \circ \mathcal{D}^2\Psi[\mathbf{A}] \left(\mathbf{k}, (\mathcal{D}\Psi[\mathbf{A}])^{-1} \left(\mathcal{D}^2\Psi[\mathbf{A}] \left(\mathbf{k}, (\mathcal{D}\Psi[\mathbf{A}])^{-1}(\mathbf{h}) \right) \right) \right) \right], \end{aligned}$$

for each $\mathbf{A} \succeq \mathbf{0}$ and $\mathbf{h}, \mathbf{k} \in \mathbb{M}_d^{sa}$;

- (f) $(\mathbf{A}, \mathbf{B}) \mapsto \text{Tr}[t\Phi(\mathbf{A}) + (1-t)\Phi(\mathbf{B}) - \Phi(t\mathbf{A} + (1-t)\mathbf{B})]$ is convex for any $0 \leq t \leq 1$;
- (g) $\mathbb{E}_1 H_\Phi(\mathbf{Z}|\mathbf{X}_1) \geq H_\Phi(\mathbb{E}_1 \mathbf{Z})$;
- (h) $\{H_\Phi(\mathbf{Z})\}_{\Phi \in (\mathcal{C}2)}$ forms a convex set of convex functions;
- (i) $H_\Phi(\mathbf{Z}) = \sup_{\mathbf{T} \succ \mathbf{0}} (\overline{\text{tr}} \mathbb{E}[(\Phi'(\mathbf{T}) - \Phi'(\mathbb{E}\mathbf{T}))(\mathbf{Z} - \mathbf{T})] + H_\Phi(\mathbf{T}))$;
- (j) $H_\Phi(\mathbf{Z}) \leq \sum_{i=1}^n \mathbb{E}H_\Phi^{(i)}(\mathbf{Z})$.

Proof. (a) \Rightarrow (i) \Rightarrow (g) \Rightarrow (j): This statement is proved by Chen and Tropp in [11].

(a) \Leftrightarrow (b): This equivalent statement is proved in [13, Theorem 2].

(a) \Leftrightarrow (d): Theorem 2.1 in [12] proved the equivalence of (a) and the following convexity lemma.

Lemma 3.1 (Convexity Lemma). [11, Lemma 4.2] Fix a function $\Phi \in \Phi_\infty$, and let $\Psi = \Phi'$. Suppose that \mathbf{A} is a random matrix taking values in \mathbb{M}_d^{++} , and let \mathbf{X} be a random matrix taking values in \mathbb{M}_d^{sa} . Assume that $\|\mathbf{A}\|, \|\mathbf{X}\|$ are integrable. Then

$$\mathbb{E}\langle \mathbf{X}, \mathcal{D}\Psi[\mathbf{A}](\mathbf{X}) \rangle \geq \langle \mathbb{E}[\mathbf{X}], \mathcal{D}\Psi[\mathbb{E}\mathbf{A}](\mathbb{E}\mathbf{X}) \rangle.$$

What remains is to establish equivalence between the convexity lemma and condition (d). This follows easily from Lemma 2.2:

$$(3.3) \quad \text{Tr}(\mathcal{D}^2\Phi[\mathbf{A}](\mathbf{X}, \mathbf{X})) = \langle \mathbf{X}, \mathcal{D}\Phi'[\mathbf{A}](\mathbf{X}) \rangle,$$

Remark 3.1. In Ref. [11, Lemma 4.2], it is shown that the concavity of the map:

$$\mathbf{A} \mapsto \left\langle \mathbf{X} (\mathcal{D}\Psi[\mathbf{A}])^{-1}(\mathbf{X}) \right\rangle, \quad \forall \mathbf{X} \in \mathbb{M}_d^{sa}$$

implies the joint convexity of the map (i.e. Lemma 3.1).

$$(3.4) \quad (\mathbf{X}, \mathbf{A}) \mapsto \langle \mathbf{X} (\mathcal{D}\Psi[\mathbf{A}])^{-1}(\mathbf{X}) \rangle.$$

In Ref. [12, Theorem 2.1], the author provided another proof for the above implication (i.e. Lemma 3.1). It is worth mentioning that the proof in [12, Theorem 2.1] originated from [46, Theorem 4.21]. Moreover, the converse direction of Lemma 3.1 follows simply from the argument in [46, Theorem 4.21]. It is also noted in [12] that the joint convexity of Eq. (3.4) indicates the entropy class Φ_∞ being a convex set. Therefore, the set of matrix Φ -entropy functionals forms a convex cone.

(b) \Leftrightarrow (c) \Leftrightarrow (d): Define $A_\Phi, B_\Phi, C_\Phi : \mathbb{M}_d^+ \times \mathbb{M}_d^+ \rightarrow \mathbb{R}$ as

$$\begin{aligned} A_\Phi(\mathbf{u}, \mathbf{v}) &\triangleq \text{Tr}[\Phi(\mathbf{u} + \mathbf{v}) - \Phi(\mathbf{u}) - \text{D}\Phi[\mathbf{u}](\mathbf{v})] \\ B_\Phi(\mathbf{u}, \mathbf{v}) &\triangleq \text{Tr}[\text{D}\Phi[\mathbf{u} + \mathbf{v}](\mathbf{v}) - \text{D}\Phi[\mathbf{u}](\mathbf{v})] \\ C_\Phi(\mathbf{u}, \mathbf{v}) &\triangleq \text{Tr}[\text{D}^2\Phi[\mathbf{u}](\mathbf{v}, \mathbf{v})]. \end{aligned}$$

Following from [9], we can establish the following relations: for any $(\mathbf{u}, \mathbf{v}) \in \mathbb{M}_d^+ \times \mathbb{M}_d^+$,

$$(3.5) \quad A_\Phi(\mathbf{u}, \mathbf{v}) = \int_0^1 (1-s) C_\Phi(\mathbf{u} + s\mathbf{v}, \mathbf{v}) ds$$

$$(3.6) \quad B_\Phi(\mathbf{u}, \mathbf{v}) = \int_0^1 C_\Phi(\mathbf{u} + s\mathbf{v}, \mathbf{v}) ds,$$

and for small enough $\epsilon > 0$,

$$(3.7) \quad A_\Phi(\mathbf{u}, \epsilon\mathbf{v}) = \frac{1}{2} C_\Phi(\mathbf{u}, \mathbf{v}) \epsilon^2 + o(\epsilon^2);$$

$$(3.8) \quad B_\Phi(\mathbf{u}, \epsilon\mathbf{v}) = C_\Phi(\mathbf{u}, \mathbf{v}) \epsilon^2 + o(\epsilon^2).$$

Eq. (3.5) is exactly the integral representation for the matrix Bréman divergence proved in [13]. Similarly, Eq. (3.6) follows from

$$\begin{aligned} B_\Phi(\mathbf{u}, \mathbf{v}) &= \frac{d}{ds} \text{Tr}[\Phi(\mathbf{u} + s\mathbf{v})] \Big|_{s=1} - \frac{d}{ds} \text{Tr}[\Phi(\mathbf{u} + s\mathbf{v})] \Big|_{s=0} \\ &= \int_0^1 \frac{d}{ds} \left(\frac{d}{ds} \text{Tr}[\Phi(\mathbf{u} + s\mathbf{v})] \right) ds \\ &= \int_0^1 C_\Phi(\mathbf{u} + s\mathbf{v}, \mathbf{v}) ds. \end{aligned}$$

Eqs. (3.7) and (3.8) can be obtained by Taylor expansion at $(\mathbf{u}, \mathbf{0})$. That is,

$$\begin{aligned} A_\Phi(\mathbf{u}, \epsilon\mathbf{v}) &= A_\Phi(\mathbf{u}, \mathbf{0}) + \text{D}_{\mathbf{u}} A_\Phi[\mathbf{u}, \mathbf{0}](\mathbf{0}) + \text{D}_{\mathbf{v}} A_\Phi[\mathbf{u}, \mathbf{0}](\epsilon\mathbf{v}) \\ &\quad + \frac{1}{2} (\text{D}_{\mathbf{u}}^2 A_\Phi[\mathbf{u}, \mathbf{0}](\mathbf{0}, \mathbf{0}) + 2\text{D}_{\mathbf{u}} \text{D}_{\mathbf{v}} A_\Phi[\mathbf{u}, \mathbf{0}](\mathbf{0}, \epsilon\mathbf{v}) + \text{D}_{\mathbf{v}}^2 A_\Phi[\mathbf{u}, \mathbf{0}](\epsilon\mathbf{v}, \epsilon\mathbf{v})) + o(\epsilon^2) \\ &= \text{Tr} \left[\text{D}\Phi[\mathbf{u} + \mathbf{0}](\epsilon\mathbf{v}) - \text{D}\Phi[\mathbf{u}](\text{D}[\mathbf{v}](\epsilon\mathbf{v})) + \frac{1}{2} \text{D}^2\Phi[\mathbf{u} + \mathbf{0}](\epsilon\mathbf{v}, \epsilon\mathbf{v}) \right] + o(\epsilon^2) \\ &= \frac{1}{2} C_\Phi(\mathbf{u}, \mathbf{v}) \epsilon^2 + o(\epsilon^2). \end{aligned}$$

Following the same argument,

$$\begin{aligned} B_\Phi(\mathbf{u}, \epsilon\mathbf{v}) &= B_\Phi(\mathbf{u}, \mathbf{0}) + \text{D}^2\Phi[\mathbf{u} + \mathbf{0}](\mathbf{0}, \epsilon\mathbf{v}) + \text{D}\Phi[\mathbf{u} + \mathbf{0}](\text{D}[\mathbf{v}](\epsilon\mathbf{v})) - \text{D}\Phi[\mathbf{u}](\text{D}[\mathbf{v}](\epsilon\mathbf{v})) \\ &\quad + \frac{1}{2} (\text{D}^3\Phi[\mathbf{u} + \mathbf{0}](\mathbf{0}, \epsilon\mathbf{v}, \epsilon\mathbf{v}) + 2\text{D}^2\Phi[\mathbf{u} + \mathbf{0}](\epsilon\mathbf{v}, \epsilon\mathbf{v})) + o(\epsilon^2) \\ &= C_\Phi(\mathbf{u}, \mathbf{v}) \epsilon^2 + o(\epsilon^2). \end{aligned}$$

We can observe from Eqs. (3.5) and (3.6) that the joint convexity of $(\mathbf{u}, \mathbf{v}) \mapsto A_\Phi(\mathbf{u}, \mathbf{v})$ and $(\mathbf{u}, \mathbf{v}) \mapsto B_\Phi(\mathbf{u}, \mathbf{v})$ follows from that of $(\mathbf{u}, \mathbf{v}) \mapsto C_\Phi(\mathbf{u}, \mathbf{v})$. In other words, we proved that conditions (d) \Rightarrow (b) and (d) \Rightarrow (c).

Conversely, Eqs. (3.7) and (3.8) show that (b) \Rightarrow (d) and condition (c) \Rightarrow (d). To be more specific, the joint convexity of $(\mathbf{u}, \mathbf{v}) \mapsto A_\Phi(\mathbf{u}, \epsilon \mathbf{v})$ implies

$$(3.9) \quad tA_\Phi(\mathbf{u}_1, \epsilon \mathbf{v}_1) + (1-t)A_\Phi(\mathbf{u}_2, \epsilon \mathbf{v}_2) \geq A_\Phi(\mathbf{u}, \epsilon \mathbf{v}),$$

for each $\mathbf{u}_1, \mathbf{u}_2, \mathbf{v}_1, \mathbf{v}_2 \in \mathbb{M}_d^+$, $t \in [0, 1]$, $\epsilon > 0$, and $\mathbf{u} \equiv t\mathbf{u}_1 + (1-t)\mathbf{u}_2$, $\mathbf{v} \equiv t\mathbf{v}_1 + (1-t)\mathbf{v}_2$. Invoking Eq. (3.7) gives

$$tA_\Phi(\mathbf{u}_1, \epsilon \mathbf{v}_1) + (1-t)A_\Phi(\mathbf{u}_2, \epsilon \mathbf{v}_2) = \frac{tC_\Phi(\mathbf{u}_1, \mathbf{v}_1) + (1-t)C_\Phi(\mathbf{u}_2, \mathbf{v}_2)}{2}\epsilon^2 + o(\epsilon^2),$$

and

$$A_\Phi(\mathbf{u}, \epsilon \mathbf{v}) = \frac{1}{2}C_\Phi(\mathbf{u}, \mathbf{v})\epsilon^2 + o(\epsilon^2).$$

Hence, Eq. (3.9) is equivalent to

$$tC_\Phi(\mathbf{u}_1, \mathbf{v}_1)\epsilon^2 + (1-t)C_\Phi(\mathbf{u}_2, \mathbf{v}_2)\epsilon^2 + o(\epsilon^2) \geq C_\Phi(\mathbf{u}, \mathbf{v})\epsilon^2 + o(\epsilon^2).$$

The joint convexity of $(\mathbf{u}, \mathbf{v}) \mapsto C_\Phi(\mathbf{u}, \epsilon \mathbf{v})$ follows by dividing by ϵ^2 on both sides and letting $\epsilon \rightarrow 0$.

The joint convexity of $(\mathbf{u}, \mathbf{v}) \mapsto B_\Phi(\mathbf{u}, \epsilon \mathbf{v})$ can be obtained in a similar way using Eq. (3.8).

(a) \Leftrightarrow (e): It is trivial if Φ is affine; hence we assume $\Phi'' > 0$. We start from the convexity of the map:

$$(3.10) \quad \mathbf{A} \mapsto -\text{Tr} \left[\mathbf{h} (\text{D}\Psi[\mathbf{A}])^{-1} (\mathbf{h}) \right], \quad \text{for all } \mathbf{h} \in \mathbb{M}_d^{sa}.$$

To ease the burden of notation, we denote $\mathsf{T}_\mathbf{A} \triangleq \text{D}\Psi[\mathbf{A}] \simeq \mathbb{C}^{d^2 \times d^2}$ and $\widehat{\mathbf{h}} \triangleq \mathbf{h} \simeq \mathbb{C}^{d^2 \times 1}$ by the isometric isomorphism between super-operators and matrices². Then Eq. (3.10) can be re-written as

$$\mathbf{A} \mapsto -\widehat{\mathbf{h}}^\dagger \cdot \mathsf{T}_\mathbf{A}^{-1} \cdot \widehat{\mathbf{h}}, \quad \text{for all } \widehat{\mathbf{h}} \in \mathbb{C}^{d^2 \times 1},$$

which is equivalent to the non-negativity of the second derivative (see Proposition 2.2):

$$\begin{aligned} -\text{D}_\mathbf{A}^2 \left[\widehat{\mathbf{h}}^\dagger \cdot \mathsf{T}_\mathbf{A}^{-1} \cdot \widehat{\mathbf{h}} \right] (\mathbf{k}, \mathbf{k}) &= -\widehat{\mathbf{h}}^\dagger \cdot \text{D}_\mathbf{A}^2 [\mathsf{T}_\mathbf{A}^{-1}] (\mathbf{k}, \mathbf{k}) \cdot \widehat{\mathbf{h}} \\ &\geq 0, \quad \text{for all } \mathbf{A} \succeq \mathbf{0}, \widehat{\mathbf{h}} \in \mathbb{C}^{d^2 \times 1}, \mathbf{k} \in \mathbb{M}_d^{sa}. \end{aligned}$$

Now, recall the chain rule of the Fréchet derivative in Proposition 2.1:

$$\begin{aligned} \text{D}\mathcal{F} \circ \mathcal{G}[\mathbf{A}](\mathbf{u}) &= \text{D}\mathcal{F}[\mathcal{G}(\mathbf{A})] (\text{D}\mathcal{G}[\mathbf{A}](\mathbf{u})); \\ \text{D}^2\mathcal{F} \circ \mathcal{G}[\mathbf{A}](\mathbf{u}, \mathbf{v}) &= \text{D}^2\mathcal{F}[\mathcal{G}(\mathbf{A})] (\text{D}\mathcal{G}[\mathbf{A}](\mathbf{v}), \text{D}\mathcal{G}[\mathbf{A}](\mathbf{v})) \\ &\quad + \text{D}\mathcal{F}[\mathcal{G}(\mathbf{A})] (\text{D}^2\mathcal{G}[\mathbf{A}](\mathbf{u}, \mathbf{v})), \end{aligned}$$

and the formula of the differentiation of the inverse function (see Lemma A.1):

$$\begin{aligned} \text{D}\mathcal{G}[\mathbf{A}]^{-1}(\mathbf{u}) &= -\mathcal{G}(\mathbf{A})^{-1} \cdot \text{D}\mathcal{G}[\mathbf{A}](\mathbf{u}) \cdot \mathcal{G}(\mathbf{A})^{-1}; \\ \text{D}^2\mathcal{G}[\mathbf{A}]^{-1}(\mathbf{u}, \mathbf{u}) &= 2\mathcal{G}(\mathbf{A})^{-1} \cdot \text{D}\mathcal{G}[\mathbf{A}](\mathbf{u}) \cdot \mathcal{G}(\mathbf{A})^{-1} \cdot \text{D}\mathcal{G}[\mathbf{A}](\mathbf{u}) \cdot \mathcal{G}(\mathbf{A})^{-1} \\ &\quad - \mathcal{G}(\mathbf{A})^{-1} \cdot \text{D}^2\mathcal{G}[\mathbf{A}](\mathbf{u}, \mathbf{u}) \cdot \mathcal{G}(\mathbf{A})^{-1}, \end{aligned}$$

we can compute the following identities by taking $\mathcal{G}[\mathbf{A}] \equiv \mathsf{T}_\mathbf{A}$, and $\mathbf{u} \equiv \mathbf{k}$:

$$\text{D}_\mathbf{A} [\mathsf{T}_\mathbf{A}^{-1}] (\mathbf{k}) = -\mathsf{T}_\mathbf{A}^{-1} \cdot \text{D}_\mathbf{A}[\mathsf{T}_\mathbf{A}](\mathbf{k}) \cdot \mathsf{T}_\mathbf{A}^{-1},$$

and

$$\begin{aligned} \text{D}_\mathbf{A} [\mathsf{T}_\mathbf{A}^{-1}] (\mathbf{k}, \mathbf{k}) &= 2 \cdot \mathsf{T}_\mathbf{A}^{-1} \cdot \text{D}_\mathbf{A}[\mathsf{T}_\mathbf{A}](\mathbf{k}) \cdot \mathsf{T}_\mathbf{A}^{-1} \cdot \text{D}_\mathbf{A}[\mathsf{T}_\mathbf{A}](\mathbf{k}) \cdot \mathsf{T}_\mathbf{A}^{-1} \\ &\quad - \mathsf{T}_\mathbf{A}^{-1} \cdot \text{D}_\mathbf{A}^2[\mathsf{T}_\mathbf{A}](\mathbf{k}, \mathbf{k}) \cdot \mathsf{T}_\mathbf{A}^{-1}. \end{aligned}$$

Therefore, we reach the expression (3.2), and statement (a) is true if and only if (3.2) holds.

²Some authors refer $\mathsf{T}_\mathbf{A}$ to the *Louville super-operator* and call $\widehat{\mathbf{h}}$ as the *vectorisation* of \mathbf{h} ; see e.g. [62, Sec. II]

Recall that in the scalar case (i.e. $d = 1$), the Fréchet derivative can be expressed as the product of the differential and the direction (see Proposition 2.6):

$$D\Psi[a]h = \Psi'(a) \cdot h.$$

Hence, Eq. (3.2) reduces to

$$\begin{aligned} & h \cdot (\Psi'(a))^{-1} \cdot \Psi'''(a) \cdot k^2 \cdot (\Psi'(a))^{-1} \cdot h \\ &= \frac{\Phi'''(a) \cdot \Phi''(a) \cdot k^2 h^2}{\Phi''(a)^2} \\ &\geq 2 \cdot h \cdot (\Psi'(a))^{-1} \cdot \Psi''(a) \cdot k \cdot (\Psi'(a))^{-1} \cdot \Psi''(a) \cdot k \cdot (\Psi'(a))^{-1} \cdot h \\ &= \frac{2\Phi'''(a)^2 \cdot k^2 h^2}{\Phi''(a)^3}. \end{aligned}$$

for all $a > 0$ and $h, k \in \mathbb{R}$. In other words, Eq. (3.2) can be viewed as a non-commutative generalisation of the classical statement: $\Phi''' \Phi'' \geq 2\Phi'''^2$.

(d) \Leftrightarrow (f): For any $t \in [0, 1]$, define $F_t : \mathbb{M}_d^+ \times \mathbb{M}_d^+ \rightarrow \mathbb{M}_d^{sa}$ as

$$F_t(\mathbf{X}, \mathbf{Y}) \triangleq t\Phi(\mathbf{X}) + (1-t)\Phi(\mathbf{Y}) - \Phi(t\mathbf{X} + (1-t)\mathbf{Y}).$$

By taking $x \equiv (\mathbf{X}, \mathbf{Y})$ and $h \equiv (\mathbf{h}, \mathbf{k})$ in Proposition 2.2, the convexity of the twice Fréchet differentiable function F_t is equivalent to

$$D^2 F_t[\mathbf{X}, \mathbf{Y}](\mathbf{h}, \mathbf{k}) \succeq \mathbf{0} \quad \forall \mathbf{X}, \mathbf{Y} \in \mathbb{M}_d^+ \quad \text{and} \quad \forall \mathbf{h}, \mathbf{k} \in \mathbb{M}_d^{sa}.$$

Then, with the help of *partial Fréchet derivative* defined in Proposition 2.3, the second-order Fréchet derivative of $F_t(\mathbf{X}, \mathbf{Y})$ can be evaluated as

$$\begin{aligned} & D^2 F_t[\mathbf{X}, \mathbf{Y}](\mathbf{h}, \mathbf{k}) \\ &= D_{\mathbf{X}}^2 F_t[\mathbf{X}, \mathbf{Y}](\mathbf{h}, \mathbf{h}) + D_{\mathbf{Y}} D_{\mathbf{X}} F_t[\mathbf{X}, \mathbf{Y}](\mathbf{h}, \mathbf{k}) \\ &\quad + D_{\mathbf{X}} D_{\mathbf{Y}} F_t[\mathbf{X}, \mathbf{Y}](\mathbf{k}, \mathbf{h}) + D_{\mathbf{Y}}^2 F_t[\mathbf{X}, \mathbf{Y}](\mathbf{k}, \mathbf{k}) \\ &= t \cdot D^2 \Phi[\mathbf{X}](\mathbf{h}, \mathbf{h}) - t^2 \cdot D^2 \Phi[t\mathbf{X} + (1-t)\mathbf{Y}](\mathbf{h}, \mathbf{h}) \\ &\quad - t(1-t) \cdot D^2 \Phi[t\mathbf{X} + (1-t)\mathbf{Y}](\mathbf{h}, \mathbf{k}) - t(1-t) \cdot D^2 \Phi[t\mathbf{X} + (1-t)\mathbf{Y}](\mathbf{k}, \mathbf{h}) \\ &\quad + (1-t) \cdot D^2 \Phi[\mathbf{Y}](\mathbf{k}, \mathbf{k}) - (1-t)^2 \cdot D^2 \Phi[t\mathbf{X} + (1-t)\mathbf{Y}](\mathbf{k}, \mathbf{k}). \end{aligned} \tag{3.11}$$

Taking trace on both sides of (3.11) and invoking Lemma 2.2, we have

$$\begin{aligned} & \text{Tr} [D^2 F_t[\mathbf{X}, \mathbf{Y}](\mathbf{h}, \mathbf{k})] \\ &= \text{Tr} [t \cdot \mathbf{h} D\Psi[\mathbf{X}](\mathbf{h}) - t^2 \cdot \mathbf{h} D\Psi[t\mathbf{X} + (1-t)\mathbf{Y}](\mathbf{h})] \\ &\quad - \text{Tr} [t(1-t) \cdot \mathbf{h} D\Psi[t\mathbf{X} + (1-t)\mathbf{Y}](\mathbf{k}) + t(1-t) \cdot \mathbf{k} D\Psi[t\mathbf{X} + (1-t)\mathbf{Y}](\mathbf{h})] \\ &\quad + \text{Tr} [(1-t) \cdot \mathbf{k} D\Psi[\mathbf{Y}](\mathbf{k}) - (1-t)^2 \cdot \mathbf{k} D^2 \Psi[t\mathbf{X} + (1-t)\mathbf{Y}](\mathbf{k})]. \end{aligned} \tag{3.12}$$

Since both the trace and the second-order Fréchet derivative are bilinear, we have the following result

$$\begin{aligned} & \text{Tr} [t^2 \cdot \mathbf{h} D\Psi[t\mathbf{X} + (1-t)\mathbf{Y}](\mathbf{h}) + t(1-t) \cdot \mathbf{k} D\Psi[t\mathbf{X} + (1-t)\mathbf{Y}](\mathbf{h})] \\ &= \langle t\mathbf{h}, D\Psi[t\mathbf{X} + (1-t)\mathbf{Y}](t\mathbf{h}) \rangle + \langle (1-t)\mathbf{k}, D\Psi[t\mathbf{X} + (1-t)\mathbf{Y}](t\mathbf{h}) \rangle \\ &= \langle t\mathbf{h} + (1-t)\mathbf{k}, D\Psi[t\mathbf{X} + (1-t)\mathbf{Y}](t\mathbf{h}) \rangle. \end{aligned} \tag{3.13}$$

Similarly,

$$\begin{aligned} & \text{Tr} [t(1-t) \cdot \mathbf{h} D\Psi[t\mathbf{X} + (1-t)\mathbf{Y}](\mathbf{k}) + (1-t)^2 \cdot \mathbf{k} D\Psi[t\mathbf{X} + (1-t)\mathbf{Y}](\mathbf{k})] \\ &= \langle t\mathbf{h} + (1-t)\mathbf{k}, D\Psi[t\mathbf{X} + (1-t)\mathbf{Y}]((1-t)\mathbf{k}) \rangle. \end{aligned} \tag{3.14}$$

Combining Eqs. (3.13) and (3.14), Eq. (3.12) can be expressed as

$$\begin{aligned} \text{Tr} [\mathbf{D}^2 \mathbf{F}_t[\mathbf{X}, \mathbf{Y}](\mathbf{h}, \mathbf{k})] &= t \cdot \langle \mathbf{h}, \mathbf{D}\Psi[\mathbf{X}](\mathbf{h}) \rangle + (1-t) \cdot \langle \mathbf{k}, \mathbf{D}\Psi[\mathbf{Y}](\mathbf{k}) \rangle \\ &\quad - \langle (t\mathbf{h} + (1-t)\mathbf{k}), \mathbf{D}\Psi[t\mathbf{X} + (1-t)\mathbf{Y}](t\mathbf{h} + (1-t)\mathbf{k}) \rangle. \end{aligned}$$

Then, it is not hard to observe that the non-negativity of $\text{Tr} [\mathbf{D}^2 \mathbf{F}_t[\mathbf{X}, \mathbf{Y}](\mathbf{h}, \mathbf{k})]$ for every $\mathbf{X}, \mathbf{Y} \in \mathbb{M}_d^+$, $\mathbf{h}, \mathbf{k} \in \mathbb{M}_d^{\text{sa}}$, and $t \in [0, 1]$ is equivalent to the joint convexity of the map

$$(\mathbf{X}, \mathbf{A}) \mapsto \langle \mathbf{X}, \mathbf{D}\Psi[\mathbf{A}](\mathbf{X}) \rangle = \text{Tr} [\mathbf{D}^2 \Phi[\mathbf{A}](\mathbf{X}, \mathbf{X})].$$

(j) \Rightarrow (g): Considering $n = 2$, the sub-additivity means that

$$H_\Phi(\mathbf{Z}) \leq \mathbb{E}_1 H_\Phi^{(2)}(\mathbf{Z}) + \mathbb{E}_2 H_\Phi^{(1)}(\mathbf{Z}).$$

Then, we have

$$\begin{aligned} \mathbb{E}_1 H_\Phi^{(2)}(\mathbf{Z}) &\geq H_\Phi(\mathbf{Z}) - \mathbb{E}_2 H_\Phi^{(1)}(\mathbf{Z}) \\ &= \mathbb{E}\Phi(\mathbf{Z}) - \Phi(\mathbb{E}\mathbf{Z}) - \mathbb{E}_2 \mathbb{E}_1 \Phi(\mathbf{Z}) + \mathbb{E}_2 \Phi(\mathbb{E}_1 \mathbf{Z}) \\ &= \mathbb{E}_2 \Phi(\mathbb{E}_1 \mathbf{Z}) - \Phi(\mathbb{E}_2 \mathbb{E}_1 \mathbf{Z}) \\ &= H_\Phi(\mathbb{E}_1 \mathbf{Z}). \end{aligned}$$

(f) \Leftrightarrow (h): Let $s \in [0, 1]$, define a pair of positive semi-definite random matrices (\mathbf{X}, \mathbf{Y}) taking values (\mathbf{x}, \mathbf{y}) with probability s and $(\mathbf{x}', \mathbf{y}')$ with probability $(1-s)$. Then the convexity of H_Φ implies that

$$(3.15) \quad H_\Phi(t\mathbf{X} + (1-t)\mathbf{Y}) \leq tH_\Phi(\mathbf{X}) + (1-t)H_\Phi(\mathbf{Y})$$

for every $t \in [0, 1]$. Now define $F_t(\mathbf{u}, \mathbf{v}) : \mathbf{M}_d^+ \times \mathbf{M}_d^+ \rightarrow \mathbb{R}$ as

$$F_t(\mathbf{u}, \mathbf{v}) \triangleq \text{Tr} [t\Phi(\mathbf{u}) + (1-t)\Phi(\mathbf{v}) - \Phi(t\mathbf{u} + (1-t)\mathbf{v})].$$

Then, it follows that

$$\begin{aligned} sF_t(\mathbf{x}, \mathbf{y}) + (1-s)F_t(\mathbf{x}', \mathbf{y}') &- F_t(s(\mathbf{x}, \mathbf{y}) + (1-s)\mathbf{x}', \mathbf{y}') \\ &= t\mathbb{E}\Phi(\mathbf{X}) - t\Phi(\mathbb{E}\mathbf{X}) + (1-t)\mathbb{E}\Phi(\mathbf{Y}) - (1-t)\Phi(\mathbb{E}\mathbf{Y}) \\ &\quad - \mathbb{E}\Phi(t\mathbf{X} + (1-t)\mathbf{Y}) + \Phi(t\mathbb{E}\mathbf{X} + (1-t)\mathbb{E}\mathbf{Y}) \\ &= tH_\Phi(\mathbf{X}) + (1-t)H_\Phi(\mathbf{Y}) - H_\Phi(t\mathbf{X} + (1-t)\mathbf{Y}), \end{aligned}$$

which means that the convexity of the pair $(\mathbf{u}, \mathbf{v}) \mapsto F_t(\mathbf{u}, \mathbf{v})$ is equivalent to the convexity of H_Φ , i.e. Eq. (3.15).

(g) \Leftrightarrow (h): Define a positive semi-definite random matrix $\mathbf{Z} \triangleq f(\mathbf{X}_1, \mathbf{X}_2)$, which depends on two random variables $\mathbf{X}_1, \mathbf{X}_2$ on a Polish space. Denote by $\mathbf{Z}_{\mathbf{X}_1}$ the random matrix \mathbf{Z} conditioned on \mathbf{X}_1 . According to the convexity of H_Φ , it follows that

$$\begin{aligned} \mathbb{E}_1 H_\Phi(\mathbf{Z}|\mathbf{X}_1) &= \mathbb{E}_1 H_\Phi(\mathbf{Z}_{\mathbf{X}_1}) \\ &= \mathbb{E}_1 \left[\overline{\text{tr}} (\mathbb{E}_2 \Phi(\mathbf{Z}_{\mathbf{X}_1}) - \Phi(\mathbb{E}_2 \mathbf{Z}_{\mathbf{X}_1})) \right] \\ &\geq \overline{\text{tr}} \mathbb{E}_2 \Phi(\mathbb{E}_1 \mathbf{Z}_{\mathbf{X}_1}) - \overline{\text{tr}} [\Phi(\mathbb{E}_1 \mathbb{E}_2 \mathbf{Z}_{\mathbf{X}_1})] \\ &= H_\Phi(\mathbb{E}_1 \mathbf{Z}). \end{aligned}$$

Conversely, define a positive semi-definite random matrix $\mathbf{Z}(s, \mathbf{X}, \mathbf{Y}) \triangleq s\mathbf{X} + (1-s)\mathbf{Y}$ where s is a random variable. Now let s be Bernoulli distributed with parameter $t \in [0, 1]$. Then for all $t \in [0, 1]$, the inequality $\mathbb{E}_1 H_\Phi(\mathbf{Z}|s) \geq H_\Phi(\mathbb{E}_1 \mathbf{Z})$ coincides

$$H_\Phi(t\mathbf{X} + (1-t)\mathbf{Y}) \leq tH_\Phi(\mathbf{X}) + (1-t)H_\Phi(\mathbf{Y}).$$

□

4. MATRIX CONCENTRATION INEQUALITIES

The main results in this section include various matrix concentration inequalities for matrix Φ -entropies. We derive *matrix Poincaré inequalities* for general multivariate super-operators $\mathcal{L} : (\mathbb{M}_{d_1}^{\text{sa}})^n \rightarrow \mathbb{M}_{d_2}^{\text{sa}}$ (Theorem 4.2), multivariate standard matrix functions (Corollary 4.1), and Lipschitz functions (Corollary 4.2) in Section 4.1. We then extend the matrix Poincaré inequality to Gaussian distribution (called *matrix Gaussian Poincaré inequality*, Theorem 4.3). These results rely on the *matrix Efron-Stein inequality*, which is first proved in [28, Theorem 4.2]. Here we re-derive a special case in Theorem 4.1 that uses the subadditivity property of matrix Φ -entropies. Its proof is, arguably, simpler.

Section 4.2 presents the results on Sobolev inequalities for matrix Φ -entropies. The *matrix Φ -Sobolev inequality* of symmetric Bernoulli random variables and that of Gaussian random variables are in Theorem 4.5 and Theorem 4.6, respectively. The *matrix logarithmic Φ -Sobolev inequality* of symmetric Bernoulli random variables and that of Gaussian random variables are in Corollaries 4.3 and 4.4.

Throughout this section, let $\mathbf{X} \triangleq (\mathbf{X}_1, \dots, \mathbf{X}_n)$ be a series of independent random variables taking values in some Polish space and let $\mathbf{Z} \triangleq \mathcal{L}(\mathbf{X}) \in \mathbb{M}_d^{\text{sa}}$ be a random matrix such that $\|\mathbb{E}\mathbf{Z}^2\|_\infty < \infty$. Let \mathbf{X}'_i be an independent copy of \mathbf{X}_i , for $1 \leq i \leq n$, and denote $\tilde{\mathbf{X}}^{(i)} \triangleq (\mathbf{X}_1, \dots, \mathbf{X}_{i-1}, \mathbf{X}'_i, \mathbf{X}_{i+1}, \dots, \mathbf{X}_n)$, i.e. replacing the i -th component of \mathbf{X} by the independent copy \mathbf{X}'_i . Let $\mathbf{X}_{-i} \triangleq (\mathbf{X}_1, \dots, \mathbf{X}_{i-1}, \mathbf{X}_{i+1}, \dots, \mathbf{X}_n)$ and $\mathbb{E}_i[\cdot] \triangleq \mathbb{E}[\cdot | \mathbf{X}_{-i}]$, i.e. expectation with respect to the i -th variable. Finally, denote by $\mathbf{Z}'_i \triangleq \mathcal{L}(\tilde{\mathbf{X}}^{(i)})$ for every $i = 1, \dots, n$.

4.1. The Matrix Poincaré Inequality. Define the quantity

$$\mathcal{E}(\mathcal{L}) \triangleq \frac{1}{2} \overline{\text{tr}} \mathbb{E} \left[\sum_{i=1}^n \left(\mathcal{L}(\mathbf{X}) - \mathcal{L}(\tilde{\mathbf{X}}^{(i)}) \right)^2 \right],$$

and we use notations $\mathcal{E}(\mathcal{L})$ and $\mathcal{E}(\mathbf{Z})$ interchangeably in the following. The quantity $\mathcal{E}(\mathbf{Z})$ has the following equivalent expressions (Lemma A.2):

$$\begin{aligned} \mathcal{E}(\mathbf{Z}) &= \frac{1}{2} \sum_{i=1}^n \overline{\text{tr}} \mathbb{E} \left[(\mathbf{Z} - \mathbf{Z}'_i)^2 \right] \\ &= \sum_{i=1}^n \overline{\text{tr}} \mathbb{E} \left[(\mathbf{Z} - \mathbb{E}_i \mathbf{Z})^2 \right] \\ &= \sum_{i=1}^n \overline{\text{tr}} \mathbb{E} \left[(\mathbf{Z} - \mathbf{Z}'_i)_+^2 \right], \end{aligned} \tag{4.1}$$

where for $\mathbf{A} \in \mathbb{M}^{\text{sa}}$, $(\mathbf{A})_+ = \sum_{i: \lambda_i > 0} \lambda_i |i\rangle\langle i|$ denotes the contribution from its positive eigenvalues. Denote the (real-valued) variance of a random matrix \mathbf{A} (taking values in \mathbb{M}_d^{sa}) by

$$\text{Var}(\mathbf{A}) \triangleq \overline{\text{tr}} \left[\mathbb{E}(\mathbf{A} - \mathbb{E}\mathbf{A})^2 \right] = \overline{\text{tr}} \left[\mathbb{E}\mathbf{A}^2 - (\mathbb{E}\mathbf{A})^2 \right].$$

Theorem 4.1 (Matrix Efron-Stein Inequality). *With the prevailing assumptions, we have*

$$\text{Var}(\mathbf{Z}) \leq \mathcal{E}(\mathbf{Z}) = \sum_{i=1}^n \overline{\text{tr}} \mathbb{E} \left[(\mathbf{Z} - \mathbf{Z}'_i)_+^2 \right]. \tag{4.2}$$

Proof. Denote $\text{Var}^{(i)}(\mathbf{Z}) \triangleq \overline{\text{tr}} \mathbb{E}_i(\mathbf{Z} - \mathbb{E}_i \mathbf{Z})^2$. Since \mathbf{Z}'_i is an independent copy of \mathbf{Z} conditioned on \mathbf{X}_{-i} , hence Lemma A.2 yields

$$\text{Var}^{(i)}(\mathbf{Z}) = \overline{\text{tr}} \mathbb{E}_i \left[(\mathbf{Z} - \mathbf{Z}'_i)_+^2 \right]. \tag{4.3}$$

With the equivalences $\text{Var}(\mathbf{Z}) = H_\Phi(\mathbf{Z})$ and $\text{Var}^{(i)}(\mathbf{Z}) = H_\Phi^{(i)}(\mathbf{Z})$, where $\Phi(u) = u^2$, this theorem is a direct consequence of the subadditivity of matrix Φ -entropies; namely, Theorem 3.2:

$$\begin{aligned}
\text{Var}(\mathbf{Z}) &\leq \sum_{i=1}^n \mathbb{E} \text{Var}^{(i)}(\mathbf{Z}) \\
&= \sum_{i=1}^n \overline{\text{tr}} \mathbb{E} \left[(\mathbf{Z} - \mathbf{Z}'_i)_+^2 \right] \\
&= \mathcal{E}(\mathbf{Z}).
\end{aligned}$$

□

The last line follows from (4.1).

Remark 4.1. Theorem 4.1 can be expressed in terms of Schatten 2-norm (see Eq. (4.2)):

$$(4.4) \quad \mathbb{E} \|\mathbf{Z} - \mathbb{E}\mathbf{Z}\|_2^2 \leq \frac{1}{2} \mathbb{E} \sum_{i=1}^n \|\mathbf{Z} - \mathbf{Z}'_i\|_2^2.$$

We remark that Paulin, Mackey, and Tropp [28, Theorem 4.2] have derived a generalised Efron-Stein inequality

$$\mathbb{E} \|\mathbf{Z} - \mathbb{E}\mathbf{Z}\|_{2p}^{2p} \leq 2(2p-1) \cdot \mathbb{E} \left\| \sum_{i=1}^n (\mathbf{Z} - \mathbf{Z}'_i)^2 \right\|_p^p.$$

which reduces to Eq. (4.4) (as $p = 1$) with a worse constant. ◇

The matrix Efron-Stein inequality can be used to prove a matrix version of the Poincaré inequality.

Theorem 4.2 (Matrix Poincaré Inequality). *Let $\mathbf{X} = (\mathbf{X}_1, \dots, \mathbf{X}_n) \in (\mathbb{M}_{d_1}^{\text{sa}})^n$ be an n -tuple independent random matrix taking values in the interval $[0, \mathbf{I}]$ (under the Löwner partial ordering) and let $\mathcal{L} : (\mathbb{M}_{d_1}^{\text{sa}}([0, 1]))^n \rightarrow \mathbb{M}_{d_2}^{\text{sa}}$ be a separately convex function³ with finite partial Fréchet derivatives. Then $\mathcal{L}(\mathbf{X}) = \mathcal{L}(\mathbf{X}_1, \dots, \mathbf{X}_n)$ satisfies*

$$\text{Var}(\mathcal{L}(\mathbf{X})) \leq \sum_{i=1}^n \mathbb{E} \left[\|\mathbf{D}_{\mathbf{X}_i} \mathcal{L}[\mathbf{X}]\|_2^2 \right],$$

where $\|\mathbf{D}_{\mathbf{X}_i} \mathcal{L}[\mathbf{X}]\|_2$ is the norm of the Fréchet derivative defined in Eq. (2.4).

Proof. Recall $\mathbf{Z} \equiv \mathcal{L}(\mathbf{X})$ and $\mathbf{Z}_i \equiv \mathcal{L}(\tilde{\mathbf{X}}^{(i)}) = \mathcal{L}(\mathbf{X}_1, \dots, \mathbf{X}_{i-1}, \mathbf{X}'_i, \mathbf{X}_{i+1}, \dots, \mathbf{X}_n)$, where \mathbf{X}'_i is an identical copy of \mathbf{X}_i . The proof follows from the matrix Efron-Stein inequality, Theorem 4.1:

$$\text{Var}(\mathcal{L}(\mathbf{X})) = \text{Var}(\mathbf{Z}) \leq \sum_{i=1}^n \overline{\text{tr}} \mathbb{E} (\mathbf{Z} - \mathbf{Z}_i)_+^2.$$

³Note that \mathcal{L} here is a multivariate super-operator. The separate convexity means that, for $0 \leq t \leq 1$,

$$t\mathcal{L}(\mathbf{Y}) + (1-t)\mathcal{L}(\tilde{\mathbf{Y}}^{(i)}) \preceq \mathcal{L}(t\mathbf{Y} + (1-t)\tilde{\mathbf{Y}}^{(i)})$$

for $\mathbf{Y} = (\mathbf{Y}_1, \dots, \mathbf{Y}_n) \in (\mathbb{M}_d^{\text{sa}})^n$, and $\tilde{\mathbf{Y}}^{(i)} = (\mathbf{Y}_1, \dots, \mathbf{Y}_{i-1}, \mathbf{Y}'_i, \mathbf{Y}_{i+1}, \dots, \mathbf{Y}_n) \in (\mathbb{M}_d^{\text{sa}})^n$.

Then it suffices to bound each term $\overline{\text{tr}} \mathbb{E} (\mathbf{Z} - \mathbf{Z}_i)_+^2$ of the right-hand side above:

$$\begin{aligned}
\overline{\text{tr}} (\mathbf{Z} - \mathbf{Z}_i)_+^2 &= \overline{\text{tr}} \left(\mathcal{L}(\mathbf{X}) - \mathcal{L}(\tilde{\mathbf{X}}^{(i)}) \right)_+^2 \\
&\leq \overline{\text{tr}} \left(\mathbf{D}_{\mathbf{X}_i} \mathcal{L}[\mathbf{X}] (\mathbf{X}_i - \mathbf{X}'_i) \right)_+^2 \\
&\leq \overline{\text{tr}} \left| \mathbf{D}_{\mathbf{X}_i} \mathcal{L}[\mathbf{X}] (\mathbf{X}_i - \mathbf{X}'_i) \right|^2 \\
&= \left\| \mathbf{D}_{\mathbf{X}_i} \mathcal{L}[\mathbf{X}] (\mathbf{X}_i - \mathbf{X}'_i) \right\|_2^2 / d_2 \\
&\leq \left\| \mathbf{D}_{\mathbf{X}_i} \mathcal{L}[\mathbf{X}] \right\|_2^2 \cdot \left\| \mathbf{X}_i - \mathbf{X}'_i \right\|_2^2 / d_2 \\
&\leq \left\| \mathbf{D}_{\mathbf{X}_i} \mathcal{L}[\mathbf{X}] \right\|_2^2 \cdot \left\| \mathbf{I} \right\|_2^2 / d_2 \\
&= \left\| \mathbf{D}_{\mathbf{X}_i} \mathcal{L}[\mathbf{X}] \right\|_2^2.
\end{aligned}$$

The second line comes from the separate operator convexity of \mathcal{L} :

$$(4.5) \quad \mathcal{L}(\mathbf{X}) - \mathcal{L}(\tilde{\mathbf{X}}^{(i)}) \preceq \mathbf{D}_{\mathbf{X}_i} \mathcal{L}[\mathbf{X}] (\mathbf{X}_i - \mathbf{X}'_i),$$

and the monotonicity of the trace function composed of the monotone function $(\cdot)_+^2$ (see Proposition 2.4). The next line follows from the relation

$$\mathbf{A}_+ \preceq |\mathbf{A}|, \quad \forall \mathbf{A} \in \mathbb{M}^{\text{sa}}.$$

The fourth line follows from the definition of Schatten 2-norm (2.1) (i.e. Frobenius norm):

$$\|\cdot\|_2 \triangleq (\text{Tr} |\cdot|^2)^{\frac{1}{2}}.$$

The fifth line follows directly from the norm of Fréchet derivatives, i.e.

$$\|\mathbf{D}f[\mathbf{A}](\mathbf{B})\|_2 \leq \|\mathbf{D}f[\mathbf{A}]\|_2 \cdot \|\mathbf{B}\|_2, \quad \forall \mathbf{A}, \mathbf{B} \in \mathbb{M}^{\text{sa}}.$$

Finally, we use the assumption $\mathbf{0} \preceq \mathbf{X}_i, \mathbf{X}'_i \preceq \mathbf{I}$ and $\|\mathbf{I}\|_2 = \sqrt{d_2}$ to complete the proof. \square

Note that Theorem 4.2 generalises the classical Poincaré inequality (e.g. [5, Theorem 3.17]):

$$\text{Var}(f(X)) \leq \mathbb{E} \left[\|\nabla f(X)\|^2 \right],$$

where $X \triangleq (X_1, \dots, X_n)$ denotes an independent random vector; each element takes values in the interval $[0, 1]$.

Remark 4.2. We remark that although the matrix Poincaré inequality and its classical counterpart have similar expressions, their proof techniques are different. The proof of classical Poincaré inequality relies on an infimum representation of $Z_i \equiv \inf_{x'_i} f(X_1, \dots, x'_i, \dots, X_n)$ in the Efron-Stein inequality in Eq. (??) (see e.g. [24, 25]). The reason for choosing such a Z_i is to guarantee the (almost surely) non-negativity of $Z - Z_i$ so that the square function preserves the ordering of the inequality, i.e.

$$\begin{aligned}
0 &\leq f(X) - f(\tilde{X}^{(i)}) \leq \frac{\partial f(X)}{\partial x_i} (X_i - X'_i) \\
\Rightarrow \quad &\left(f(X) - f(\tilde{X}^{(i)}) \right)^2 \leq \left(\frac{\partial f(X)}{\partial x_i} (X_i - X'_i) \right)^2.
\end{aligned}$$

However, the matrix version of Poincaré inequality is more intricate; namely, the infimum may not exist in the range of a matrix-valued function $\mathcal{L}(\mathbf{X})$. Such a difficulty can be circumvented by considering $(\mathcal{L}(\mathbf{X}) - \mathcal{L}(\tilde{\mathbf{X}}^{(i)}))_+$; hence the separable operator convexity (4.5) cannot be applied. \diamond

Note that Theorem 4.2 considers the matrix Poincaré inequality for general matrix functions $\mathcal{L} : (\mathbb{M}_d^{\text{sa}})^n \rightarrow \mathbb{M}_d^{\text{sa}}$, while in Corollary 4.1 below, we impose additional pairwise commutative criteria on $\mathbf{X} = (\mathbf{X}_1, \dots, \mathbf{X}_n)$; namely, $[\mathbf{X}_i, \mathbf{X}_j] = \mathbf{0}$ almost surely for $i \neq j \in [n]$, we can have the following Matrix Poincaré inequality for *multivariate standard matrix functions* (Definition 2.2).

Corollary 4.1 (Matrix Poincaré Inequality for Multivariate Standard Matrix Functions). *Let $\mathbf{X} = (\mathbf{X}_1, \dots, \mathbf{X}_n)$ be an n -tuple independent random matrix taking values in \mathbb{S}_d^n with joint spectrum in $[0, 1]^n$, i.e. $[\mathbf{X}_i, \mathbf{X}_j] = \mathbf{0}$ almost surely for $i \neq j \in [n]$. Let $f : ([0, 1]^n) \rightarrow \mathbb{R}$ be a multivariate standard matrix function that is separately operator convex and has finite partial Fréchet derivatives. Then, $f(\mathbf{X}) = f(\mathbf{X}_1, \dots, \mathbf{X}_n)$ satisfies*

$$\text{Var}(f(\mathbf{X})) \leq \sum_{i=1}^n \mathbb{E} \left\| [\varphi_i(\bar{\lambda}_k, \bar{\lambda}_\ell)]_{k\ell} \right\|_{\text{sup}}^2,$$

where φ_i is the divided difference of f defined in Eq. (2.4), and $\bar{\lambda}_k \triangleq (\lambda_{1k}, \dots, \lambda_{ik}, \dots, \lambda_{nk})$ with λ_{ik} being the i -th eigenvalue of \mathbf{X}_k .

Proof. Following the same argument in the proof of Theorem 4.2, we have

$$\begin{aligned} \overline{\text{tr}}(\mathbf{Z} - \mathbf{Z}_i)_+^2 &\leq \|\mathbf{D}_{\mathbf{X}_i} f[\mathbf{X}] (\mathbf{X}_i - \mathbf{X}'_i)\|_2^2 / d \\ &= \|[\varphi_i(\bar{\lambda}_k, \bar{\lambda}_\ell)]_{k\ell} \odot (\mathbf{X}_i - \mathbf{X}'_i)\|_2^2 / d \\ &\leq \|[\varphi_i(\bar{\lambda}_k, \bar{\lambda}_\ell)]_{k\ell}\|_{\text{sup}}^2 \cdot \|\mathbf{X}_i - \mathbf{X}'_i\|_2^2 / d \\ &\leq \|[\varphi_i(\bar{\lambda}_k, \bar{\lambda}_\ell)]_{k\ell}\|_{\text{sup}}^2 \cdot \|\mathbf{I}\|_2^2 / d \\ &= \|[\varphi_i(\bar{\lambda}_k, \bar{\lambda}_\ell)]_{k\ell}\|_{\text{sup}}^2, \end{aligned}$$

where the second line follows from the multivariate version of Daleckiĭ and Kreĭn formula (2.7). In the third line we apply the norm inequality for the Schur product [63], i.e.

$$\|\mathbf{A} \odot \mathbf{B}\|_2 \leq \|\mathbf{A}\|_{\text{sup}} \cdot \|\mathbf{B}\|_2, \quad \forall \mathbf{A}, \mathbf{B} \in \mathbb{M}.$$

□

Remark 4.3. It is worth mentioning that Corollary 4.1 also reduces back to the classical Poincaré inequality for real-valued functions ($d = 1$) and for vector-valued functions (corresponding to $(\mathbf{X}_i)_{i=1}^n$ being $d \times d$ diagonal random matrices). Hence, Theorem 4.2 is essentially a “non-commutative” generalisation of classical Poincaré inequality while Corollary 4.1 is a “commutative” generalisation. ◇

If the multivariate standard matrix function f is a Lipschitz function with the Lipschitz constant

$$\|f\|_\Lambda \triangleq \sup \frac{|f(\bar{x}) - f(\bar{y})|}{\|\bar{x} - \bar{y}\|_1},$$

where $\bar{x} = (x_1, \dots, x_n) \in \mathbb{R}^n$, then the matrix Poincaré inequality (Corollary 4.1) has an even more appealing form.

Corollary 4.2 (Matrix Poincaré Inequality for Lipschitz Functions). *Let $\mathbf{X} = (\mathbf{X}_1, \dots, \mathbf{X}_n)$ be an n -tuple of independent random matrices taking values in \mathbb{S}_d^n with joint spectrum in $[0, 1]^n$, i.e. $[\mathbf{X}_i, \mathbf{X}_j] = \mathbf{0}$ almost surely for $i \neq j \in [n]$. Let $f : ([0, 1]^n) \rightarrow \mathbb{R}$ be a multivariate standard matrix function with Lipschitz constant $\|f\|_\Lambda$. Then for all n -tuples of random matrices \mathbf{X} , there exists a universal constant $k(n)$ such that*

$$\text{Var}(f(\mathbf{X})) \leq k(n) \|f\|_\Lambda^2.$$

Proof. The main ingredient to establish this corollary is to use the following bound for Lipschitz functions.

Proposition 4.1 ([64]). *Let $\mathbf{A} = (\mathbf{A}_i)_{i=1}^n$ and $\mathbf{B} = (\mathbf{B}_i)_{i=1}^n$ be families of commuting self-adjoint operators. If $f : \mathbb{R}^n \rightarrow \mathbb{C}$ is a Lipschitz function, then there exists a constant $k'(n)$,*

$$\|f(\mathbf{A}) - f(\mathbf{B})\|_p \leq k'(n) \|f\|_\Lambda \sum_{i=1}^n \|\mathbf{A}_i - \mathbf{B}_i\|_p.$$

It follows that

$$\begin{aligned}
\overline{\text{tr}} \left[f(\mathbf{X}) - f(\tilde{\mathbf{X}}_i) \right]^2 &= \frac{1}{d} \left\| f(\mathbf{X}) - f(\tilde{\mathbf{X}}_i) \right\|_2^2 \\
&\leq \frac{1}{d} \left(k'(n) \|f\|_\Lambda \cdot \left(\|\mathbf{X} - \mathbf{X}_i\|_2 + \sum_{j \neq i} \|\mathbf{X}_j - \mathbf{X}_j\|_2 \right) \right)^2 \\
&\leq \frac{1}{d} k'(n)^2 \cdot \|f\|_\Lambda^2 \|\mathbf{I}\|_2^2 \\
&= k'(n)^2 \cdot \|f\|_\Lambda^2,
\end{aligned}$$

and therefore

$$\begin{aligned}
\text{Var}(f(\mathbf{X})) &\leq \sum_{i=1}^n \mathbb{E} \overline{\text{tr}} \left[f(\mathbf{X}) - f(\tilde{\mathbf{X}}_i) \right]^2 \\
&\leq \frac{k'(n)^2}{2} \sum_{i=1}^n \|f\|_\Lambda^2 \\
&= k(n) \|f\|_\Lambda^2
\end{aligned}$$

where, in the last line, $k(n) \equiv n \frac{k'(n)^2}{2}$. \square

The significance of the subadditivity property can be seen in Corollary 4.2 when the function is a Lipschitz function. The resulting Poincaré inequality only depends the Lipschitz constant and a universal constant $k(n)$.

Remark 4.4. A multivariate function f is called *operator Lipschitz* if there exists a universal constant C ,

$$\|f(\mathbf{A}) - f(\mathbf{B})\| \leq C \cdot \max_{1 \leq i \leq n} \|\mathbf{A}_i - \mathbf{B}_i\|$$

for all n -tuple commuting self-adjoint operators $(\mathbf{A}_i)_{i=1}^n$ and $(\mathbf{B}_i)_{i=1}^n$. It was proved that not every Lipschitz function f is operator Lipschitz [65]. \diamond

The matrix Efron-Stein inequality is used in Theorem 4.2 to prove the matrix Poincaré inequality. Next we will show that the matrix Efron-Stein can be also applied to establish an upper bound, known as the *Gaussian Poincaré inequality*, for a Fréchet differentiable matrix-valued function of *Gaussian Unitary Ensembles (GUE)*⁴.

Theorem 4.3 (Matrix Gaussian Poincaré Inequality). *Let $\mathbf{X}_1, \dots, \mathbf{X}_n$ be independent random matrices⁵ from the Gaussian Unitary Ensemble and let $\mathcal{L} : (\mathbb{M}_{d_1}^{\text{sa}})^n \rightarrow \mathbb{M}_{d_2}^{\text{sa}}$ be any twice Fréchet differentiable function. Then $\mathcal{L}(\mathbf{X})$ satisfies*

$$\text{Var}(\mathcal{L}(\mathbf{X})) \leq \sum_{i=1}^n \mathbb{E} \left[\left\| \mathbf{D}_{\mathbf{X}_i} \mathcal{L}[\mathbf{X}] \right\|_2^2 \right].$$

Proof. We borrow the idea from [67] (see also [5, Theorem 3.20]) to prove this theorem. First, we assume $\sum_{i=1}^n \mathbb{E} \left[\left\| \mathbf{D}_{\mathbf{X}_i} \mathcal{L}[\mathbf{X}] \right\|_2^2 \right] \leq \infty$; otherwise the inequality holds trivially. Second, it suffices to establish the theorem for $n = 1$:

$$(4.6) \quad \text{Var}(\mathcal{L}(\mathbf{X})) \leq \mathbb{E} \left[\left\| \mathbf{D} \mathcal{L}[\mathbf{X}] \right\|_2^2 \right].$$

It can be easily extended to every $n \in \mathbb{N}$ by applying the matrix Efron-Stein inequality, Theorem 4.1.

⁴The Gaussian Unitary Ensembles are a family of random Hermitian matrices whose upper-triangular entries are independently and identically distributed (i.i.d.) complex standard Gaussian random variables, while the diagonal entries are i.i.d. real standard Gaussian random variables; see e.g. [66, §2.6]

⁵We consider “entry-wise” independence here.

Now for every $j \in [m] \triangleq \{1, \dots, m\}$, denote by $\mathbf{W}_j, \mathbf{W}'_j$ the $d_1 \times d_1$ matrices whose entries are sampled from independent Rademacher random variables (i.e. uniformly $\{\pm 1\}$ -valued random variables) and let

$$\mathbf{Y}_j = \frac{(\mathbf{W}_j + \mathbf{i} \cdot \mathbf{W}'_j) + (\mathbf{W}_j + \mathbf{i} \cdot \mathbf{W}'_j)^\dagger}{2}.$$

Let $\epsilon_1, \dots, \epsilon_m$ be a series of independent Rademacher random variables, and define

$$\mathbf{S}_m \triangleq \frac{1}{\sqrt{m}} \sum_{j=1}^m \epsilon_j \mathbf{Y}_j.$$

Then, for every $j \in [m]$,

$$\text{Var}^{(j)}(\mathcal{L}(\mathbf{S}_m)) = \frac{1}{4} \overline{\text{tr}} \left[\left(\mathcal{L} \left(\mathbf{S}_m + \frac{1 - \epsilon_j}{\sqrt{m}} \mathbf{Y}_j \right) - \mathcal{L} \left(\mathbf{S}_m - \frac{1 + \epsilon_j}{\sqrt{m}} \mathbf{Y}_j \right) \right)^2 \right].$$

Invoke the matrix Efron-Stein inequality to obtain

$$(4.7) \quad \text{Var}(\mathcal{L}(\mathbf{S}_m)) = \frac{1}{4} \sum_{j=1}^m \overline{\text{tr}} \mathbb{E} \left[\left(\mathcal{L} \left(\mathbf{S}_m + \frac{1 - \epsilon_j}{\sqrt{m}} \mathbf{Y}_j \right) - \mathcal{L} \left(\mathbf{S}_m - \frac{1 + \epsilon_j}{\sqrt{m}} \mathbf{Y}_j \right) \right)^2 \right].$$

Now we use Taylor expansion to further bound the right-hand side of Eq. (4.7). For every $i \in [n]$ and some constants $0 \leq \alpha, \beta \leq 1$, it follows almost surely that

$$\begin{aligned} \mathcal{L} \left(\mathbf{S}_m + \frac{1 - \epsilon_j}{\sqrt{m}} \mathbf{Y}_j \right) &= \mathcal{L}(\mathbf{S}_m) + \text{D}\mathcal{L}[\mathbf{S}_m] \left(\frac{1 - \epsilon_j}{\sqrt{m}} \mathbf{Y}_j \right) + \mathcal{R}_2 \left(\mathbf{S}_m, \frac{1 - \epsilon_j}{\sqrt{m}} \mathbf{Y}_j \right); \\ \mathcal{L} \left(\mathbf{S}_m - \frac{1 + \epsilon_j}{\sqrt{m}} \mathbf{Y}_j \right) &= \mathcal{L}(\mathbf{S}_m) + \text{D}\mathcal{L}[\mathbf{S}_m] \left(-\frac{1 + \epsilon_j}{\sqrt{m}} \mathbf{Y}_j \right) + \mathcal{R}_2 \left(\mathbf{S}_m, -\frac{1 + \epsilon_j}{\sqrt{m}} \mathbf{Y}_j \right), \end{aligned}$$

where $\mathcal{R}_l : \mathbb{M}_{d_1} \times \mathbb{M}_{d_1} \rightarrow \mathbb{M}_{d_2}$ is the remainder term of the Taylor series:

$$\mathcal{R}_l(\mathbf{X}, \mathbf{E}) \triangleq \sum_{k=l}^{\infty} \frac{1}{k!} \text{D}^k \mathcal{L}[\mathbf{X}] (\underbrace{\mathbf{E}, \dots, \mathbf{E}}_k) = o(|\mathbf{E}|^l).$$

Therefore,

$$\mathcal{L} \left(\mathbf{S}_m + \frac{1 - \epsilon_j}{\sqrt{m}} \mathbf{Y}_j \right) - \mathcal{L} \left(\mathbf{S}_m - \frac{1 + \epsilon_j}{\sqrt{m}} \mathbf{Y}_j \right) \preceq \frac{2}{\sqrt{m}} \text{D}\mathcal{L}[\mathbf{S}_m] (\mathbf{Y}_j) + o\left(\frac{1}{m}\right),$$

and

$$\begin{aligned} & \frac{1}{4} \sum_{j=1}^m \overline{\text{tr}} \mathbb{E} \left[\left(\mathcal{L} \left(\mathbf{S}_m + \frac{1 - \epsilon_j}{\sqrt{m}} \mathbf{Y}_j \right) - \mathcal{L} \left(\mathbf{S}_m - \frac{1 + \epsilon_j}{\sqrt{m}} \mathbf{Y}_j \right) \right)^2 \right] \\ & \leq \|\text{D}\mathcal{L}[\mathbf{S}_m]\|_2^2 + o\left(\frac{1}{\sqrt{m}}\right). \end{aligned}$$

Let m go to infinity, we have

$$(4.8) \quad \lim_{m \rightarrow \infty} \frac{1}{4} \sum_{i=1}^m \overline{\text{tr}} \mathbb{E} \left[\left(\mathcal{L} \left(\mathbf{S}_m + \frac{1 - \epsilon_j}{\sqrt{m}} \mathbf{Y}_j \right) - \mathcal{L} \left(\mathbf{S}_m - \frac{1 + \epsilon_j}{\sqrt{m}} \mathbf{Y}_j \right) \right)^2 \right] = \mathbb{E} \left[\|\text{D}\mathcal{L}[\mathbf{X}]\|_2^2 \right],$$

where by the central limit theorem (see Lemma A.3) that \mathbf{S}_m converges in distribution to a random matrix \mathbf{X} in GUE. Thus $\text{Var}(\mathcal{L}(\mathbf{S}_m))$ converges to $\text{Var}(\mathcal{L}(\mathbf{X}))$.

Finally, the subadditivity of the variance and Eq. (4.6) lead to

$$\begin{aligned}\text{Var}(\mathcal{L}(\mathbf{X})) &\leq \sum_{i=1}^n \mathbb{E} \left[\text{Var}^{(i)}(\mathcal{L}(\mathbf{X})) \right] \\ &\leq \sum_{i=1}^n \mathbb{E} \left[\mathbb{E}_i \left[\|\mathbf{D}_{\mathbf{X}_i} \mathcal{L}[\mathbf{X}]\|_2^2 \right] \right] \\ &= \sum_{i=1}^n \mathbb{E} \left[\|\widehat{\mathbf{D}}_{\mathbf{X}_i} \mathcal{L}[\mathbf{X}]\|_2^2 \right],\end{aligned}$$

which completes the proof. \square

4.2. Matrix Φ -Sobolev Inequalities. For completeness, we provide a short review of the classical *Bonami-Beckner inequality* in Appendix B.

In this section, we consider matrix-valued functions defined on Boolean hypercubes: $\mathbf{f} : \{0, 1\} \rightarrow \mathbb{M}_d^{\text{sa}}$ and establish matrix Φ -Sobolev inequalities. The main ingredient to prove this inequality comes from Fourier analysis and the hypercontractive inequality for matrix-valued functions.

Ben-Aroya *et al.* [18] generalised Bonami and Beckner's results by considering matrix-valued functions $\mathbf{f} : \{0, 1\} \rightarrow \mathbb{M}_d$. Similarly, Fourier analysis can be naturally extended into the matrix setting; that is, the Fourier transform $\widehat{\mathbf{f}}$ of the matrix-valued function \mathbf{f} can be expressed as

$$\begin{cases} \widehat{\mathbf{f}}(S) = \frac{1}{2^n} \sum_{x \in \{0, 1\}^n} \mathbf{f}(x) \chi_S(x); \\ \mathbf{f}(x) = \sum_{S \subseteq \{1, \dots, n\}} \widehat{\mathbf{f}}(S) \chi_S(x), \end{cases}$$

Therefore, the hypercontractive inequality (B.2) can be extended to matrix-valued functions.

Theorem 4.4 (Matrix Bonami-Beckner Inequality [18]). *For every $\mathbf{f} : \{0, 1\}^n \rightarrow \mathbb{M}_d$ and $1 \leq p \leq 2$,*

$$\left(\sum_{S \subseteq [n]} (p-1)^{|S|} \|\widehat{\mathbf{f}}(S)\|_{*p}^2 \right)^{1/2} \leq \left(\frac{1}{2^n} \sum_{x \in \{0, 1\}^n} \|\mathbf{f}(x)\|_{*p}^p \right)^{1/p},$$

where the normalised Schatten p -norm is defined as $\|\mathbf{M}\|_{*p} = (\overline{\text{tr}} |\mathbf{M}|^p)^{1/p}$ for $\mathbf{M} \in \mathbb{M}_d$.

With Theorem 4.4, we can prove a matrix Φ -Sobolev inequality for matrix-valued functions defined on symmetric Bernoulli random variables.

Theorem 4.5 (Matrix Φ -Sobolev Inequalities for Symmetric Bernoulli Random Variables). *Let X be uniformly distributed over $\mathcal{X} \equiv \{0, 1\}^n$ (an n -dimensional binary hypercube) and $\mathbf{f} : \mathcal{X} \rightarrow \mathbb{M}_d^+$ be an arbitrary matrix-valued function. Then for all $p \in (1, 2)$, and $\Phi(u) = u^{2/p}$,*

$$(4.9) \quad H_\Phi(\mathbf{f}^p) \leq (2-p)\mathcal{E}(\mathbf{f}) \cdot d^{1-2/p} + \overline{\text{tr}} \mathbb{E}[\mathbf{f}^2] \cdot (1 - d^{1-2/p}).$$

Proof. Starting from the left-hand side of Eq. (4.9), the definition of the matrix Φ -entropy functional gives that

$$\begin{aligned}(4.10) \quad H_\Phi(\mathbf{f}^p) &= \overline{\text{tr}} \mathbb{E}[\mathbf{f}^2] - \overline{\text{tr}} \left[(\mathbb{E} \mathbf{f}^p)^{2/p} \right] \\ &\leq \overline{\text{tr}} \mathbb{E}[\mathbf{f}^2] - (\overline{\text{tr}} \mathbb{E} \mathbf{f}^p)^{2/p} \\ &= \overline{\text{tr}} \mathbb{E}[\mathbf{f}^2] - (\overline{\text{tr}} \mathbb{E} |\mathbf{f}|^p)^{2/p} \quad (\text{since } \mathbf{f}(X) \succ \mathbf{0}) \\ &= \overline{\text{tr}} \mathbb{E}[\mathbf{f}^2] - \left(\mathbb{E} \|\mathbf{f}\|_{*p}^p \right)^{2/p},\end{aligned}$$

where we apply the convexity lemma of normalised trace function (Lemma 2.1) and recall that $(\cdot)^{2/p}$ is a convex function for $1 \leq p \leq 2$.

Next, since the Schatten p -norm is a non-increasing function of p , we have the following relation for the normalised Schatten p -norm

$$\begin{aligned}
\|\mathbf{M}\|_{*p}^2 &= (\overline{\text{tr}} |\mathbf{M}|^p)^{2/p} \\
&= (\text{Tr} |\mathbf{M}|^p)^{2/p} \cdot d^{-2/p} \\
&\geq (\text{Tr} |\mathbf{M}|^2)^{2/2} \cdot d^{-2/p} \\
&= (\overline{\text{tr}} |\mathbf{M}|^2) \cdot d^{1-2/p} \\
&= \|\mathbf{M}\|_{*2}^2 \cdot d^{1-2/p},
\end{aligned}
\tag{4.11}$$

for every $\mathbf{M} \in \mathbb{M}_d$ and $1 \leq p \leq 2$. Then, by combining Eq. (4.11) and Theorem 4.4, Eq. (4.10) can be rewritten as

$$\begin{aligned}
H_\Phi(\mathbf{f}^p) &\leq \overline{\text{tr}} \mathbb{E} [\mathbf{f}^2] - \left(\mathbb{E} \|\mathbf{f}\|_{*p}^p \right)^{2/p} \\
&\leq \overline{\text{tr}} \mathbb{E} [\mathbf{f}^2] - \left(\sum_{S \subseteq [n]} (p-1)^{|S|} \left\| \widehat{\mathbf{f}}(S) \right\|_{*p}^2 \right)^{2/p} \\
&= \overline{\text{tr}} \mathbb{E} [\mathbf{f}^2] - \left(\sum_{S \subseteq [n]} (p-1)^{|S|} \overline{\text{tr}} [\widehat{\mathbf{f}}(S)^2] \right)^{2/p} \cdot d^{1-2/p} \\
&= \overline{\text{tr}} \left[\sum_{S \subseteq [n]} \widehat{\mathbf{f}}(S)^2 \right] - \left(\sum_{S \subseteq [n]} (p-1)^{|S|} \overline{\text{tr}} [\widehat{\mathbf{f}}(S)^2] \right)^{2/p} \cdot d^{1-2/p} \\
&= \overline{\text{tr}} \left[\sum_{S \subseteq [n]} \left(1 - (p-1)^{|S|} d^{1-2/p} \right) \widehat{\mathbf{f}}(S)^2 \right],
\end{aligned}
\tag{4.12}$$

where we apply Parseval's identity (Lemma A.4) in the fourth line.

From the elementary analysis, it holds for all $S \subseteq [n]$ and $1 \leq p \leq 2$,

$$1 - (p-1)^{|S|} \leq (2-p)|S|.$$

Therefore, it follows that

$$1 - (p-1)^{|S|} d^{1-2/p} \leq (2-p)|S| d^{1-2/p} + (1 - d^{1-2/p}).$$

Finally, by using the fact that $\sum_{S \subseteq [n]} \overline{\text{tr}} [|\mathbf{f}| \widehat{\mathbf{f}}(S)^2] = \mathcal{E}(\mathbf{f})$ (see Lemma A.5), Eq. (4.12) can be further deduced as

$$\begin{aligned}
H_\Phi(\mathbf{f}^p) &\leq \overline{\text{tr}} \left[\sum_{S \subseteq [n]} \left(1 - (p-1)^{|S|} d^{1-2/p} \right) \widehat{\mathbf{f}}(S)^2 \right] \\
&\leq \overline{\text{tr}} \left[\sum_{S \subseteq [n]} \left((2-p)|S| d^{1-2/p} + (1 - d^{1-2/p}) \right) \widehat{\mathbf{f}}(S)^2 \right] \\
&= (2-p) \mathcal{E}(\mathbf{f}) \cdot d^{1-2/p} + \overline{\text{tr}} \left[\sum_{S \subseteq [n]} \widehat{\mathbf{f}}(S)^2 \cdot (1 - d^{1-2/p}) \right] \\
&= (2-p) \mathcal{E}(\mathbf{f}) \cdot d^{1-2/p} + \overline{\text{tr}} \mathbb{E} [\mathbf{f}^2] \cdot (1 - d^{1-2/p}),
\end{aligned}$$

which completes our claim. \square

Theorem 4.6 (Matrix Φ -Sobolev Inequalities for Gaussian Distributions). *Let $X = (X_1, \dots, X_n)$ be a vector of n independent standard Gaussian random variables taking values in $\mathcal{X} \equiv \mathbb{R}^n$, and let $\mathbf{f} : \mathcal{X} \rightarrow \mathbb{M}_d^+$ be an arbitrary matrix-valued function. Then for all $p \in (1, 2)$, and $\Phi(u) = u^{2/p}$,*

$$(4.13) \quad H_\Phi(\mathbf{f}^p) \leq (2-p) \sum_{i=1}^n \mathbb{E} \left[\|\mathbf{D}_{\mathbf{X}_i} \mathbf{f}[\mathbf{X}]\|_2^2 \right] \cdot d^{1-2/p} + \overline{\text{tr}} \mathbb{E}[\mathbf{f}^2] \cdot (1 - d^{1-2/p}).$$

Proof. The proof parallels the approach in Theorem 4.3. Denote

$$\mathcal{E}^{(i)}(\mathbf{f}) \triangleq \frac{1}{2} \overline{\text{tr}} \mathbb{E}_i \left[\sum_{j=1}^n \left(\mathbf{f}(X) - \mathbf{f}(\tilde{X}^{(i)}) \right)^2 \right],$$

and

$$\mathcal{E}(\mathbf{f}) = \sum_{i=1}^n \mathbb{E} \left[\mathcal{E}^{(i)}(\mathbf{f}) \right].$$

Recall from Eq. (4.8) and let $\mathbf{Y}_i \equiv 1$:

$$\mathcal{E}^{(i)}(\mathbf{f}) = \lim_{m \rightarrow \infty} \frac{1}{4} \sum_{j=1}^m \overline{\text{tr}} \mathbb{E}_i \left[\left(\mathbf{f} \left(S_m + \frac{1-\epsilon_i}{\sqrt{m}} \right) - \mathbf{f} \left(S_m - \frac{1+\epsilon_i}{\sqrt{m}} \right) \right)^2 \right] = \mathbb{E}_i \left[\|\mathbf{D}_{\mathbf{X}_i} \mathbf{f}[\mathbf{X}]\|_2^2 \right].$$

This and Theorem (4.5) yield Eq. (4.6) and the statement follows. \square

The logarithmic Sobolev inequality for matrix-valued functions immediately follows from Theorems 4.5 and 4.6.

Corollary 4.3 (Matrix Logarithmic Sobolev Inequalities for Symmetric Bernoulli Random Variables). *Let $\mathbf{f} : \{0, 1\}^n \rightarrow \mathbb{M}_d^+$ be an arbitrary matrix-valued function defined on the n -dimensional binary hypercube and assume that X is uniformly distributed over $\{0, 1\}^n$. Then*

$$\text{Ent}(\mathbf{f}^2) \leq 2\mathcal{E}(\mathbf{f}) + \log(d) \cdot \overline{\text{tr}} \mathbb{E}[\mathbf{f}^2].$$

Proof. By letting $p \rightarrow 2$, the left-hand side of Eq. (4.9) becomes

$$\lim_{p \rightarrow 2^-} \frac{H_\Phi(\mathbf{f}^p)}{2-p} = \lim_{p \rightarrow 2^-} \frac{\overline{\text{tr}} \left[\mathbb{E}[\mathbf{f}(X)^2] - \left(\mathbb{E}[\mathbf{f}(X)^p]^{2/p} \right) \right]}{2-p} = \frac{\text{Ent}(\mathbf{f}^2)}{2},$$

where the last identity follows from Lemma A.6. Similarly, the right-hand side gives

$$\lim_{p \rightarrow 2^-} \frac{(2-p)\mathcal{E}(\mathbf{f}) \cdot d^{1-2/p} + \overline{\text{tr}} \mathbb{E}[\mathbf{f}^2] \cdot (1 - d^{1-2/p})}{2-p} = \mathcal{E}(\mathbf{f}) + \frac{\log(d)}{2} \cdot \overline{\text{tr}} \mathbb{E}[\mathbf{f}^2]$$

as established. \square

Corollary 4.4 (Matrix Gaussian Logarithmic Sobolev Inequalities). *Assume that X is a vector of independent and identical standard Gaussian random variables on \mathbb{R}^n and let $\mathbf{f} : \mathbb{R}^n \rightarrow \mathbb{M}_d^+$ be an arbitrary matrix-valued function of X . Then*

$$\text{Ent}(\mathbf{f}^2) \leq 2 \sum_{i=1}^n \mathbb{E} \left[\|\mathbf{D}_{\mathbf{X}_i} \mathbf{f}[\mathbf{X}]\|_2^2 \right] + \log(d) \cdot \overline{\text{tr}} \mathbb{E}[\mathbf{f}^2].$$

Remark 4.5. Denoted by $\text{LS}(C, D)$ (see e.g. [68, Section 5.1]) the set of logarithmic Sobolev inequalities with constants $C > 0$, $D \geq 0$:

$$\text{Ent}(f^2) \leq 2C\mathcal{E}(f) + D\mathbb{E}[f^2].$$

When $D = 0$, the logarithmic Sobolev inequality is called *tight*; otherwise, it is called *defective*. It is well known that the best constants of the classical logarithmic Sobolev inequalities for symmetric Bernoulli random variables and standard Gaussian random variables are $(C, D) = (1, 0)$ [15, 69]. However, numerical simulation shows that examples ($d > 1$) exist for matrix-valued functions so that: $\text{Ent}(\mathbf{f}^2) > 2\mathcal{E}(\mathbf{f})$. In Corollary 4.3, we establish the logarithmic Sobolev inequality with constant $(C, D) = (1, \log d)$. \diamond

5. ENTROPIC INEQUALITY FOR CLASSICAL-QUANTUM ENSEMBLES

In this section, we connect the matrix Φ -entropies with quantum information theory and present a functional inequality for the classical-quantum (c-q) ensembles that undergo a special Markov evolution.

Let \mathcal{X} be a sample space. We denote by $\mathcal{P}(\mathcal{X})$ the set of all probability distributions on \mathcal{X} and by $\mathcal{P}_*(\mathcal{X})$ the subset of $\mathcal{P}(\mathcal{X})$ which consists of all strictly positive distributions. The set of all $d \times d$ matrix-valued functions on \mathcal{X} is denoted by $\mathcal{F}(\mathcal{X})$; $\mathcal{F}_*(\mathcal{X})$ and $\mathcal{F}_*^0(\mathcal{X})$ are the subsets of $\mathcal{F}(\mathcal{X})$ consisting of all strictly positive and non-negative functions, respectively.

Any *classical discrete channel* or *Markov kernel* with input alphabet \mathcal{X} and output alphabet \mathcal{Y} can be described by a transition probabilities $\{K(y|x) : x \in \mathcal{X}, y \in \mathcal{Y}\}$. For any probability distribution μ defined on the alphabet \mathcal{X} , we denote the channel acting on μ from the right by

$$(5.1) \quad \mu K(y) \triangleq \sum_{x \in \mathcal{X}} \mu(x) K(y|x), \quad y \in \mathcal{Y},$$

or acting on matrix-valued functions $\mathbf{f} \in \mathcal{F}(\mathcal{Y})$ by

$$(5.2) \quad K \mathbf{f}(x) \triangleq \sum_{y \in \mathcal{Y}} K(y|x) \mathbf{f}(y), \quad x \in \mathcal{X}.$$

The set of all classical channels is denoted by $\mathcal{M}(\mathcal{Y}|\mathcal{X})$. If $\mu \otimes K \in \mathcal{P}(\mathcal{X}) \times \mathcal{M}(\mathcal{Y}|\mathcal{X})$ denotes the distribution of a random pair $(X, Y) \in \mathcal{X} \times \mathcal{Y}$ with $P_X = \mu$ and $P_{Y|X} = K$, then

$$(5.3) \quad K \mathbf{f}(x) = \mathbb{E}[\mathbf{f}(Y)|X = x]$$

for any $\mathbf{f} \in \mathcal{F}(\mathcal{Y})$ and $x \in \mathcal{X}$. We say that a pair $(\mu, K) \in \mathcal{P}(\mathcal{X}) \times \mathcal{M}(\mathcal{Y}|\mathcal{X})$ is *admissible* if $\mu \in \mathcal{P}_*(\mathcal{X})$ and $\mu K \in \mathcal{P}_*(\mathcal{Y})$. Hence the *backward* or *adjoint* channel $K^* \in \mathcal{M}(\mathcal{X}|\mathcal{Y})$ can be defined by

$$(5.4) \quad K^*(x|y) = \frac{K(y|x)\mu(x)}{\mu K(y)}, \quad (x, y) \in \mathcal{X} \times \mathcal{Y}.$$

If $(X, Y) \sim \mu \times K$, then $K^* = P_{X|Y}$ and

$$(5.5) \quad K^* \mathbf{f}(y) = \mathbb{E}[\mathbf{f}(X)|Y = y]$$

for any $\mathbf{f} \in \mathcal{F}(\mathcal{X})$ and $y \in \mathcal{Y}$.

Recall that the conditional matrix Φ -entropy of \mathbf{Z} given Y which takes values in any Polish space can be defined by

$$(5.6) \quad H_\Phi(\mathbf{Z}|Y) \triangleq \overline{\text{tr}} \mathbb{E}[\Phi(\mathbf{Z})|Y] - \overline{\text{tr}}[\Phi(\mathbb{E}[\mathbf{Z}|Y])].$$

Combining the definition of matrix Φ -entropies with (5.6) immediately gives the following law of total variance:

$$(5.7) \quad \begin{aligned} H_\Phi(\mathbf{Z}) &= \overline{\text{tr}} \mathbb{E}[\Phi(\mathbf{Z})] - \overline{\text{tr}}[\Phi(\mathbb{E}[\mathbf{Z}])] \\ &= \overline{\text{tr}} \mathbb{E}_Y \mathbb{E}[\Phi(\mathbf{Z})] - \overline{\text{tr}}[\Phi(\mathbb{E}_Y \mathbb{E}[\mathbf{Z}|Y])] \\ &= \mathbb{E}_Y [H_\Phi(\mathbf{Z}|Y) + \overline{\text{tr}} \Phi(\mathbb{E}[\mathbf{Z}|Y])] - \overline{\text{tr}}[\Phi(\mathbb{E}_Y \mathbb{E}[\mathbf{Z}|Y])] \\ &= \mathbb{E}_Y [H_\Phi(\mathbf{Z}|Y)] + H_\Phi(\mathbb{E}[\mathbf{Z}|Y]). \end{aligned}$$

Fix $\Phi(u) = u \log u$ and assume that the distribution $\mu \in \mathcal{P}(\mathcal{X})$ is defined on a discrete space \mathcal{X} . If we consider a random matrix $\boldsymbol{\rho}_X$ to be an ensemble of classical-quantum (c-q) states $(\mu, \boldsymbol{\nu}) \triangleq \{(\mu(x), \boldsymbol{\rho}_x)\}_{x \in \mathcal{X}}$, where each $\boldsymbol{\rho}_x \succeq 0$ and $\text{Tr} \boldsymbol{\rho}_x = 1$, then its Φ -entropy is related to the *Holevo quantity* of $\{(\mu(x), \boldsymbol{\rho}_x)\}_{x \in \mathcal{X}}$:

$$\begin{aligned} d \cdot H_\Phi(\boldsymbol{\rho}_X) &\equiv \sum_{x \in \mathcal{X}} \mu(x) \text{Tr}[\boldsymbol{\rho}_x \log \boldsymbol{\rho}_x] - \text{Tr}[\bar{\boldsymbol{\rho}} \log \bar{\boldsymbol{\rho}}] \\ &= \sum_{x \in \mathcal{X}} \mu(x) \cdot S(\boldsymbol{\rho}_x \| \bar{\boldsymbol{\rho}}) \\ &=: \chi(\mu, \boldsymbol{\nu}), \end{aligned}$$

where $\bar{\boldsymbol{\rho}} = \mathbb{E}_\mu[\boldsymbol{\rho}_X] = \sum_{x \in \mathcal{X}} \mu(x) \boldsymbol{\rho}_x$ and $S(\boldsymbol{\rho} \| \boldsymbol{\sigma}) \triangleq \text{Tr} \boldsymbol{\rho}(\log \boldsymbol{\rho} - \log \boldsymbol{\sigma})$ is the quantum relative entropy.

Denote by $\rho_Y \equiv \{\mu'(y), \rho'_y\}_{y \in \mathcal{Y}}$ the resulting random matrix of ρ_X that undergoes a Markov evolution K by the rule:

$$(5.8) \quad \{\mu(x)\}_{x \in \mathcal{X}} \mapsto \{\mu K(y)\}_{y \in \mathcal{Y}} = \left\{ \sum_{x \in \mathcal{X}} \mu(x) K(y|x) \right\}_{y \in \mathcal{Y}} =: \{\mu'(y)\}_{y \in \mathcal{Y}};$$

$$(5.9) \quad \{\rho_x\}_{x \in \mathcal{X}} \mapsto \{K^* \nu(y)\}_{y \in \mathcal{Y}} = \left\{ \sum_{x \in \mathcal{X}} K^*(x|y) \rho_x \right\}_{y \in \mathcal{Y}} =: \{\rho'_y\}_{y \in \mathcal{Y}}.$$

Note that each ρ'_y can be interpreted as the conditional expectation $\mathbb{E}_{K^*}[\rho_X|Y=y]$, which is a post-selection state with the probability law $\{K^*(x|y)\}_{x \in \mathcal{X}}$. We also have the following relation between the Φ -entropy of ρ_Y and the Holevo quantity of $(\mu', \nu') \triangleq \{\mu'(y), \rho'_y\}_{y \in \mathcal{Y}}$:

$$(5.10) \quad d \cdot H_\Phi(\rho_Y) = \sum_{y \in \mathcal{Y}} \mu'(y) \text{Tr} [\rho'_y \log \rho'_y] - \text{Tr} [\bar{\rho}' \log \bar{\rho}']$$

$$(5.11) \quad =: \chi(\mu', \nu'),$$

where $\bar{\rho}' = \mathbb{E}_{\mu'}[\rho_Y] = \sum_{y \in \mathcal{Y}} \mu'(y) \rho'_y$.

Now for any $\mu \in \mathcal{P}(\mathcal{X})$ and $K \in \mathcal{M}(Y|X)$, we define the constant:

$$(5.12) \quad \eta_\Phi(\mu, K) \triangleq \sup_{\nu \neq \mu \mathbf{I}} \frac{\chi(\mu', \nu')}{\chi(\mu, \nu)}.$$

By Jensen's inequality, it can be shown that $0 \leq \eta_\Phi(\mu, K) \leq 1$ (see Lemma A.7). Therefore, we relate $\eta_\Phi(\mu, K)$ to the following functional inequality of the matrix Φ -entropies:

Proposition 5.1 (Functional Form for C-Q Ensembles). *Fix an admissible pair (μ, K) and let (X, Y) be a random pair with probability law $\mu \otimes K$. Then $\eta_\Phi(\mu, K) \leq c$ if and only if the inequality*

$$(5.13) \quad H_\Phi[\mathbf{f}(X)] \leq \frac{1}{1-c} \mathbb{E} (H_\Phi[\mathbf{f}(X)|Y])$$

holds for all non-constant classical-quantum states $\mathbf{f} : \mathcal{X} \rightarrow \mathcal{Q}(\mathbb{C}^d)$, where we denote by $\mathcal{Q}(\mathbb{C}^d)$ all the density operators on \mathbb{C}^d . In particular, Eq. (5.13) can be expressed in terms of Holevo quantities:

$$(5.14) \quad \chi(\mu, \nu) \leq \frac{1}{1-c} \mathbb{E}_Y [\chi(K^*, \nu|Y)]$$

where the expectation \mathbb{E}_Y is taken with respect to $\{\mu K(y)\}_{y \in \mathcal{Y}}$.

Moreover,

$$(5.15) \quad \eta_\Phi(\mu, K) = 1 - \inf \left\{ \frac{\mathbb{E} [H_\Phi(\mathbf{f}(X)|Y)]}{H_\Phi(\mathbf{f}(X))} : \mathbf{f} \neq \text{const} \right\}.$$

Proof. The inequality $\chi(\mu', \nu') \leq c \cdot \chi(\mu, \nu)$ is equivalent to

$$(5.16) \quad \begin{aligned} H_\Phi(K^* \mathbf{f}(Y)) &\leq c H_\Phi(\mathbf{f}(X)) \\ &= c (\mathbb{E} [H_\Phi(\mathbf{f}(X)|Y)] + H_\Phi(\mathbb{E} [\mathbf{f}(X)|Y])) \\ &= c (\mathbb{E} [H_\Phi(\mathbf{f}(X)|Y)] + H_\Phi(K^* \mathbf{f}(Y))) \end{aligned}$$

where we use the identity of the law of total variance, Eq. (5.7), and the property of the backward channel, Eq. (5.5), from which we obtain

$$(5.17) \quad H_\Phi(K^* \mathbf{f}(Y)) \leq \frac{c}{1-c} \mathbb{E} [H_\Phi(\mathbf{f}(X)|Y)],$$

and hence,

$$(5.18) \quad \begin{aligned} H_\Phi[\mathbf{f}(X)] &= \mathbb{E} [H_\Phi(\mathbf{f}(X)|Y)] + H_\Phi(K^* \mathbf{f}(Y)) \\ &\leq \frac{1}{1-c} \mathbb{E} (H_\Phi[\mathbf{f}(X)|Y]). \end{aligned}$$

□

Raginsky showed, in recent work [26, 27], that if $f = d\nu/d\mu$ (i.e. a Radon-Nikodym derivative), then

$$(5.19) \quad K^* f = \frac{d(\nu K)}{d(\mu K)}.$$

Moreover, the constant $\eta_\Phi(\mu, K)$ in Eq. (5.12) corresponds to the (classical) *strong data processing inequality* (SDPI):

$$(5.20) \quad \eta_\Phi(\mu, K) \triangleq \sup_{\nu \neq \mu} \frac{D(\nu K, \mu K)}{D(\nu, \mu)},$$

where $D(\nu, \mu)$ is the classical Kullback-Leibler divergence of μ and ν . We remark that Proposition 5.1 will recover Raginsky's SDPI result by letting $d = 1$.

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APPENDIX A. MISCELLANEOUS LEMMAS

Lemma A.1 (Second-Order Fréchet Derivative of Inversion Function). *Let $\mathcal{G} : \mathbb{M} \rightarrow \mathbb{M}$ be second-order Fréchet differentiable at $\mathbf{A} \in \mathbb{M}$, and $\mathcal{G}(\mathbf{A})$ be invertible. Then, for each $\mathbf{h}, \mathbf{k} \in \mathbb{M}$, we have*

$$\begin{aligned} D\mathcal{G}[\mathbf{A}]^{-1}(\mathbf{h}) &= -\mathcal{G}(\mathbf{A})^{-1} \cdot D\mathcal{G}[\mathbf{A}](\mathbf{h}) \cdot \mathcal{G}(\mathbf{A})^{-1}; \\ D^2\mathcal{G}[\mathbf{A}]^{-1}(\mathbf{h}, \mathbf{k}) &= 2 \cdot \mathcal{G}(\mathbf{A})^{-1} \cdot D\mathcal{G}[\mathbf{A}](\mathbf{k}) \cdot \mathcal{G}(\mathbf{A})^{-1} \cdot D\mathcal{G}[\mathbf{A}](\mathbf{h}) \cdot \mathcal{G}(\mathbf{A})^{-1} \\ &\quad - \mathcal{G}(\mathbf{A})^{-1} \cdot D^2\mathcal{G}[\mathbf{A}](\mathbf{h}, \mathbf{k}) \cdot \mathcal{G}(\mathbf{A})^{-1}. \end{aligned}$$

Proof. Denote $\mathcal{F} : \mathbf{A} \mapsto \mathbf{A}^{-1}$ as the inversion function and recall the chain rule of the Fréchet derivative:

$$\begin{aligned} D\mathcal{F} \circ \mathcal{G}[\mathbf{A}](\mathbf{h}) &= D\mathcal{F}[\mathcal{G}(\mathbf{A})] (D\mathcal{G}[\mathbf{A}](\mathbf{h})); \\ D^2\mathcal{F} \circ \mathcal{G}[\mathbf{A}](\mathbf{h}, \mathbf{k}) &= D^2\mathcal{F}[\mathcal{G}(\mathbf{A})] (D\mathcal{G}[\mathbf{A}](\mathbf{k}), D\mathcal{G}[\mathbf{A}](\mathbf{h})) + D\mathcal{F}[\mathcal{G}(\mathbf{A})] (D^2\mathcal{G}[\mathbf{A}](\mathbf{h}, \mathbf{k})) \end{aligned}$$

It follows that

$$\begin{aligned} D\mathcal{G}[\mathbf{A}]^{-1}(\mathbf{h}) &= D\mathcal{F} \circ \mathcal{G}[\mathbf{A}](\mathbf{h}) \\ &= D\mathcal{F}[\mathcal{G}(\mathbf{A})] (D\mathcal{G}[\mathbf{A}](\mathbf{h})) \\ &= -\mathcal{G}(\mathbf{A})^{-1} \cdot D\mathcal{G}[\mathbf{A}](\mathbf{h}) \cdot \mathcal{G}(\mathbf{A})^{-1}, \end{aligned}$$

where we use the formula of the Fréchet derivative of the inversion function in the last equation; see Eq. (2.2):

$$D[\mathbf{X}]^{-1}(\mathbf{Y}) = -\mathbf{X}^{-1}\mathbf{Y}\mathbf{X}^{-1}$$

(by taking $\mathbf{X} \equiv \mathcal{G}(\mathbf{A})$ and $\mathbf{Y} \equiv D\mathcal{G}[\mathbf{A}](\mathbf{h})$).

Furthermore,

$$\begin{aligned} D^2\mathcal{G}[\mathbf{A}]^{-1}(\mathbf{h}, \mathbf{k}) &= D^2\mathcal{F} \circ \mathcal{G}[\mathbf{A}](\mathbf{h}, \mathbf{k}) \\ &= D^2\mathcal{F}[\mathcal{G}(\mathbf{A})] (D\mathcal{G}[\mathbf{A}](\mathbf{k}), D\mathcal{G}[\mathbf{A}](\mathbf{h})) + D\mathcal{F}[\mathcal{G}(\mathbf{A})] (D^2\mathcal{G}[\mathbf{A}](\mathbf{h}, \mathbf{k})) \\ &= 2 \cdot \mathcal{G}(\mathbf{A})^{-1} \cdot D\mathcal{G}[\mathbf{A}](\mathbf{k}) \cdot \mathcal{G}(\mathbf{A})^{-1} \cdot D\mathcal{G}[\mathbf{A}](\mathbf{h}) \cdot \mathcal{G}(\mathbf{A})^{-1} \\ &\quad - \mathcal{G}(\mathbf{A})^{-1} \cdot D^2\mathcal{G}[\mathbf{A}](\mathbf{h}, \mathbf{k}) \cdot \mathcal{G}(\mathbf{A})^{-1}. \end{aligned}$$

Again, we use the formula of the second-order Fréchet derivative (see e.g. [46, Exercise 3.27]):

$$D^2[\mathbf{X}]^{-1}(\mathbf{Y}_1, \mathbf{Y}_2) = \mathbf{X}^{-1}\mathbf{Y}_1\mathbf{X}^{-1}\mathbf{Y}_2\mathbf{X}^{-1} + \mathbf{X}^{-1}\mathbf{Y}_2\mathbf{X}^{-1}\mathbf{Y}_1\mathbf{X}^{-1}$$

(by taking $\mathbf{X} \equiv \mathcal{G}(\mathbf{A})$, and $\mathbf{Y}_1 \equiv \mathbf{Y}_2 \equiv D\mathcal{G}[\mathbf{A}](\mathbf{h})$).

□

Lemma A.2. Let \mathbf{X} be a random matrix taking values in \mathbb{M}^{sa} , and let \mathbf{Y} be independently and identically distributed as \mathbf{X} . Then for each natural number $q \geq 1$,

$$(A.1) \quad \mathbb{E}[|\mathbf{X} - \mathbb{E}\mathbf{X}|^q] = \mathbb{E}[(\mathbf{X} - \mathbb{E}\mathbf{X})_+^q] + \mathbb{E}[(\mathbf{X} - \mathbb{E}\mathbf{X})_-^q]$$

and

$$(A.2) \quad \frac{1}{2} \mathbb{E}[|\mathbf{X} - \mathbf{Y}|^q] = \mathbb{E}[(\mathbf{X} - \mathbf{Y})_+^q] = \mathbb{E}[(\mathbf{X} - \mathbf{Y})_-^q]$$

In particular,

$$(A.3) \quad \mathbb{E}[(\mathbf{X} - \mathbb{E}\mathbf{X})^2] = \frac{1}{2} \mathbb{E}[(\mathbf{X} - \mathbf{Y})^2].$$

Proof. For each realization X of \mathbf{X} in \mathbb{M}^{sa} , $X = X_+ - X_-$ for some $X_+, X_- \succeq 0$ and $X_+ X_- = \mathbf{0}$. Slightly abusing the notation, we hence write \mathbf{X}_+ and \mathbf{X}_- to denote the positive and negative decomposition of their realizations of \mathbf{X} .

Therefore, for each natural number $q \geq 1$,

$$\begin{aligned} \mathbb{E}[|\mathbf{X} - \mathbb{E}\mathbf{X}|^q] &= \mathbb{E}[(\mathbf{X} - \mathbb{E}\mathbf{X})_+^q + (\mathbf{X} - \mathbb{E}\mathbf{X})_-^q] \\ &= \mathbb{E}[(\mathbf{X} - \mathbb{E}\mathbf{X})_+^q] + \mathbb{E}[(\mathbf{X} - \mathbb{E}\mathbf{X})_-^q] \\ &= \mathbb{E}[(\mathbf{X} - \mathbb{E}\mathbf{X})_+^q] + \mathbb{E}[(\mathbf{X} - \mathbb{E}\mathbf{X})_-^q]. \end{aligned}$$

Likewise, we have

$$\begin{aligned} \frac{1}{2} \mathbb{E}[|\mathbf{X} - \mathbf{Y}|^q] &= \frac{1}{2} \mathbb{E}[(\mathbf{X} - \mathbf{Y})_+^q + (\mathbf{Y} - \mathbf{X})_+^q] \\ &= \frac{1}{2} \mathbb{E}[(\mathbf{X} - \mathbf{Y})_+^q] + \frac{1}{2} \mathbb{E}[(\mathbf{Y} - \mathbf{X})_+^q] \\ &= \frac{1}{2} \mathbb{E}[(\mathbf{X} - \mathbf{Y})_+^q] + \frac{1}{2} \mathbb{E}[(\mathbf{Y} - \mathbf{X})_+^q] \\ &= \mathbb{E}[(\mathbf{X} - \mathbf{Y})_+^q]. \end{aligned}$$

The last line follows since \mathbf{Y} is an identical copy of \mathbf{X} .

Following the same reasoning, we have $|\mathbf{X}| = \mathbf{X}_+ + (-\mathbf{X})_-$, and thus $\frac{1}{2} \mathbb{E}[|\mathbf{X} - \mathbf{Y}|^q] = \mathbb{E}[(\mathbf{X} - \mathbf{Y})_-^q]$. Finally, Eq. (A.3) follows from elementary calculations:

$$\begin{aligned} \frac{1}{2} \mathbb{E}[(\mathbf{X} - \mathbf{Y})^2] &= \frac{1}{2} \mathbb{E}[\mathbf{X}^2 - \mathbf{X}\mathbf{Y} - \mathbf{Y}\mathbf{X} + \mathbf{Y}^2] \\ &= \frac{1}{2} [\mathbb{E}\mathbf{X}^2 - \mathbb{E}\mathbf{X} \cdot \mathbb{E}\mathbf{Y} - \mathbb{E}\mathbf{Y} \cdot \mathbb{E}\mathbf{X} + \mathbb{E}\mathbf{Y}^2] \\ &= \mathbb{E}\mathbf{X}^2 - (\mathbb{E}\mathbf{X})^2 \\ &= \mathbb{E}[(\mathbf{X} - \mathbb{E}\mathbf{X})^2]. \end{aligned}$$

□

Lemma A.3 (Central Limit Theorem of Gaussian Unitary Ensembles). Let $\{\epsilon_j\}_j$ be a series of Rademacher variables, and let $\{\mathbf{W}_j\}_j, \{\mathbf{W}'_j\}_j$ be $d \times d$ matrices whose entries are sampled independently from the Rademacher variables. Let

$$\mathbf{Y}_j = \frac{(\mathbf{W}_j + \mathbf{i} \cdot \mathbf{W}'_j) + (\mathbf{W}_j + \mathbf{i} \cdot \mathbf{W}'_j)^\dagger}{2},$$

and

$$\mathbf{S}_m \triangleq \frac{1}{\sqrt{m}} \sum_{j=1}^m \epsilon_j \mathbf{Y}_j$$

where $\{\epsilon_j\}_j$ are Rademacher variables again. If m tends to infinity, then \mathbf{S}_m converges in distribution to a $d \times d$ matrix in the Gaussian unitary ensemble.

Proof. It is clear from the central limit theorem that the diagonal entries converge to a standard real Gaussian variable, while the upper-triangular entries converge to a complex Gaussian variables with zero mean and unit variance. Next, we show that the correlation between any (non-identical) entry vanishes as m goes to infinity. That is, for every $(k, l) \neq (k', l')$

$$\mathbb{E}_{\epsilon_1, \dots, \epsilon_m} \left[S_m^{(kl)} S_m^{(k'l')} \right] = \frac{1}{m} \sum_{j=1}^m Y_j^{(kl)} Y_j^{(k'l')},$$

from which we apply the strong law of large numbers to obtain

$$\lim_{m \rightarrow \infty} \frac{1}{m} \sum_{j=1}^m Y_j^{(kl)} Y_j^{(k'l')} = \mathbb{E} [Y \cdot Y'] = \mathbb{E} [Y] \cdot \mathbb{E} [Y'] = 0 \quad \text{almost surely,}$$

where we denote by Y (resp. Y') the random variable that the sequences $\{Y_j^{(kl)}\}_j$ (resp. $\{Y_j^{(k'l')}\}_j$) are sampled from. It is easy to see that Y and Y' are independent zero-mean random variables. Therefore, the entries are mutually independent and $\lim_{m \rightarrow \infty} S_m$ belongs to the Gaussian unitary ensemble. \square

Lemma A.4 (Parseval's Identity for Matrix-Valued Functions). *For every matrix-valued function $\mathbf{f} : \{0, 1\}^n \rightarrow \mathbb{M}_d$, we have the following identity*

$$\mathbb{E} [\mathbf{f}(X)^2] = \sum_{S \subseteq [n]} \widehat{\mathbf{f}}(S)^2,$$

where the expectation is taken uniformly over all $x \in \{0, 1\}^n$.

Proof. With the Fourier expansion of the matrix-valued function \mathbf{f} , it follows that

$$\begin{aligned} \mathbb{E} [\mathbf{f}(X)^2] &= \mathbb{E} \left[\mathbf{f}(X) \cdot \left(\sum_{S \subseteq [n]} \widehat{\mathbf{f}}(S) \chi_S(X) \right) \right] \\ &= \sum_{S \subseteq [n]} \widehat{\mathbf{f}}(S) \cdot \mathbb{E} [\mathbf{f}(X) \chi_S(X)] \\ &= \sum_{S \subseteq [n]} \widehat{\mathbf{f}}(S)^2. \end{aligned}$$

\square

Lemma A.5. *With the prevailing assumptions, and every $\mathbf{f} : \{0, 1\}^n \rightarrow \mathbb{M}_d^{sa}$, we have*

$$\sum_{S \subseteq [n]} \overline{\text{tr}} \left[|S| \widehat{\mathbf{f}}(S)^2 \right] = \mathcal{E}(\mathbf{f}).$$

Proof. For every n -tuple $x \triangleq (x_1, \dots, x_n) \in \{0, 1\}^n$, denote $\overline{x}^{(i)} \triangleq (x_1, \dots, x_{i-1}, 1 - x_i, x_{i+1}, \dots, x_n)$. For every $i \in [n]$, introduce the matrix-valued function

$$\mathbf{g}_i(x) = \frac{\mathbf{f}(x) - \mathbf{f}(\overline{x}^{(i)})}{2}.$$

Then, for every $S \subseteq [n]$, it can be observed that

$$\begin{aligned} \widehat{\mathbf{g}}_i(S) &= \mathbb{E} [\mathbf{g}_i(X) \chi_S(X)] \\ &= \frac{1}{2} \mathbb{E} \left[\left(\mathbf{f}(X) - \mathbf{f}(\overline{X}^{(i)}) \right) \cdot (-1)^{\sum_{j \in S} X_j} \right] = \begin{cases} 0 & \text{if } i \notin S \\ \widehat{\mathbf{f}}(S) & \text{if } i \in S. \end{cases} \end{aligned}$$

Apply Parseval's identity, Lemma A.4 to obtain

$$\mathbb{E} [\mathbf{g}_i(X)^2] = \sum_{S \subseteq [n]} \widehat{\mathbf{g}}_i(S)^2 = \sum_{S: i \in S} \widehat{\mathbf{f}}(S)^2.$$

Finally, since X is uniformly distributed, $\mathcal{E}(\mathbf{f})$ can be rewritten as

$$\begin{aligned}
\mathcal{E}(\mathbf{f}) &= \frac{1}{2} \overline{\text{tr}} \mathbb{E} \left[\sum_{i=1}^n \left(\mathbf{f}(X) - \mathbf{f}(\tilde{X}^{(i)}) \right)^2 \right] \\
&= \frac{1}{4} \overline{\text{tr}} \mathbb{E} \left[\sum_{i=1}^n \left(\mathbf{f}(X) - \mathbf{f}(\overline{X}^{(i)}) \right)^2 \right] \\
&= \sum_{i=1}^n \overline{\text{tr}} \mathbb{E} [\mathbf{g}_i(X)^2] \\
&= \sum_{i=1}^n \sum_{S: i \in S} \overline{\text{tr}} [\hat{\mathbf{f}}(S)^2] \\
&= \sum_{S \subseteq [n]} \overline{\text{tr}} [|S| \hat{\mathbf{f}}(S)^2].
\end{aligned}$$

This completes the proof. \square

Lemma A.6. Let \mathbf{Z} be a random matrix taking values in \mathbb{M}^+ such that $\|\mathbf{Z}\|_\infty < \infty$. For $p \in [1, 2)$, we define the matrix-valued p -variance of \mathbf{Z} by

$$\mathbf{Var}_p[\mathbf{Z}] \triangleq \mathbb{E}[\mathbf{Z}^2] - \left(\mathbb{E}[\mathbf{Z}^p] \right)^{2/p}.$$

It follows that

$$\lim_{p \rightarrow 2^-} \frac{\mathbf{Var}_p[\mathbf{Z}]}{2-p} = \frac{1}{2} \mathbb{E}[\mathbf{Z}^2 \log \mathbf{Z}^2] - \frac{1}{2} \mathbb{E}[\mathbf{Z}^2] \cdot \log \mathbb{E}[\mathbf{Z}^2].$$

Proof. We first prove a formula for the matrix differentiation. Denote by $\mathbf{A} = \mathbf{A}(p)$ a Hermitian matrix which depends on the real parameter p . Then we aim to solve the derivative of $\mathbf{A}^{2/p}$ with respect to p . Let $\mathbf{Y} = \mathbf{A}^{2/p}$. Then $\log \mathbf{Y} = \log \mathbf{A} \cdot 2/p$. Differentiating on both sides with respect to p and applying the chain rule of the Fréchet derivatives (see Proposition 2.1), the above expression leads to

$$\begin{aligned}
\frac{d}{dp} \log \mathbf{Y} &= \int_0^\infty (s\mathbf{I} + \mathbf{Y})^{-1} \cdot \frac{d}{dp} \mathbf{Y} \cdot (s\mathbf{I} + \mathbf{Y})^{-1} ds \\
&= \frac{d}{dp} \log \mathbf{A} \cdot 2/p \\
&= -\frac{2}{p^2} \log \mathbf{A} + \frac{2}{p} \int_0^\infty (t\mathbf{I} + \mathbf{A})^{-1} \cdot \frac{d}{dp} \mathbf{A} \cdot (t\mathbf{I} + \mathbf{A})^{-1} dt.
\end{aligned} \tag{A.4}$$

Note that $\mathbf{T}_D(\mathbf{K}) \triangleq \int_0^\infty (s\mathbf{I} + \mathbf{D})^{-1} \mathbf{K} (s\mathbf{I} + \mathbf{D})^{-1} ds$ is called the *Bogoliubov-Kubo-Mori operator* and its inverse is well-known to be (see e.g. [70, Appendix C.2]):

$$\mathbf{T}_D^{-1}(\mathbf{L}) = \int_0^1 \mathbf{D}^s \mathbf{L} \mathbf{D}^{1-s} ds,$$

from which Eq. (A.4) yields

$$\begin{aligned}
\frac{d}{dp} \mathbf{Y} &= \int_0^1 \mathbf{Y}^s \left[-\frac{2}{p^2} \log \mathbf{A} + \frac{2}{p} \int_0^\infty (t\mathbf{I} + \mathbf{A})^{-1} \cdot \frac{d}{dp} \mathbf{A} \cdot (t\mathbf{I} + \mathbf{A})^{-1} dt \right] \mathbf{Y}^{1-s} ds \\
&= \int_0^1 \mathbf{A}^{2s/p} \left[-\frac{2}{p^2} \log \mathbf{A} + \frac{2}{p} \int_0^\infty (t\mathbf{I} + \mathbf{A})^{-1} \cdot \frac{d}{dp} \mathbf{A} \cdot (t\mathbf{I} + \mathbf{A})^{-1} dt \right] \mathbf{A}^{2/p-2s/p} ds \\
&= -\frac{2}{p^2} \mathbf{A}^{2s/p} \cdot \log \mathbf{A} + \frac{2}{p} \int_0^1 \int_0^\infty \mathbf{A}^{2s/p} (t\mathbf{I} + \mathbf{A})^{-1} \cdot \frac{d}{dp} \mathbf{A} \cdot (t\mathbf{I} + \mathbf{A})^{-1} \mathbf{A}^{2/p-2s/p} dt ds.
\end{aligned}$$

Now taking $\mathbf{A} \equiv \mathbb{E}[\mathbf{Z}^p]$, we have

$$\frac{d}{dp} \mathbf{A} = \frac{d}{dp} \mathbb{E}[\mathbf{Z}^p] = \mathbb{E}[\mathbf{Z}^p \cdot \log \mathbf{Z}],$$

and

$$(A.5) \quad \begin{aligned} \frac{d}{dp} \left(\mathbb{E}[Z^p] \right)^{2/p} &= -\frac{2}{p^2} \left(\mathbb{E}[Z^p] \right)^{2/p} \log \mathbb{E}[Z^p] \\ &\quad + \frac{2}{p} \int_0^1 \int_0^\infty \mathbf{A}^{2s/p} (t\mathbf{I} + \mathbf{A})^{-1} \cdot \mathbb{E}[Z^p \cdot \log Z] \cdot (t\mathbf{I} + \mathbf{A})^{-1} \mathbf{A}^{2/p-2s/p} dt ds. \end{aligned}$$

Finally, we are ready to prove our claim. L'Hôpital's rule implies

$$\begin{aligned} \lim_{p \rightarrow 2^-} \frac{\text{Var}_p[Z]}{2-p} &= \frac{d}{dp} \left(\mathbb{E}[Z^p] \right)^{2/p} \Big|_{p=2} \\ &= -\frac{1}{2} \mathbb{E}[Z^2] \cdot \log \mathbb{E}[Z^2] \\ &\quad + \int_0^1 \int_0^\infty \mathbf{A}^s (t\mathbf{I} + \mathbf{A})^{-1} \cdot \mathbb{E}[Z^p \cdot \log Z] \cdot (t\mathbf{I} + \mathbf{A})^{-1} \mathbf{A}^{1-s} dt ds \\ &= -\frac{1}{2} \mathbb{E}[Z^2] \cdot \log \mathbb{E}[Z^2] + \mathbb{E}[Z^2 \log Z] \\ &= \frac{1}{2} \mathbb{E}[Z^2 \log Z^2] - \frac{1}{2} \mathbb{E}[Z^2] \cdot \log \mathbb{E}[Z^2] \end{aligned}$$

completing the proof. \square

Lemma A.7. Fix sample spaces \mathcal{X} and \mathcal{Y} . For every distribution $\mu \in \mathcal{P}(\mathcal{X})$, Markov kernel $K \in \mathcal{M}(\mathcal{Y}|\mathcal{X})$ and matrix-valued function $\mathbf{f} : \mathcal{X} \rightarrow \mathbb{M}_d^+$, we have the following inequality:

$$\begin{aligned} H_\Phi(K^* \mathbf{f}) &= \overline{\text{tr}} \left[\mathbb{E}_{\mu K} [\Phi(K^* \mathbf{f})] - \Phi(\mathbb{E}_{\mu K} [K^* \mathbf{f}]) \right] \\ &\leq \overline{\text{tr}} \left[\mathbb{E}_\mu \Phi(\mathbf{f}) - \Phi(\mathbb{E}_\mu \mathbf{f}) \right] \\ &= H_\Phi(\mathbf{f}), \end{aligned}$$

where μK and K^* are defined in Eqs. (5.1) and (5.4).

Proof. We first observe that Jensen's inequality [71, Section 5] holds for all convex function Φ :

$$(A.6) \quad \overline{\text{tr}} [K^* \Phi(\mathbf{f})] \geq \overline{\text{tr}} [\Phi(K^* \mathbf{f})].$$

After taking expectation with respect to μK , direct calculation shows that (note that we freely interchange the order of trace and expectation by Fubini's theorem):

$$\begin{aligned} \overline{\text{tr}} \mathbb{E}_{\mu K} [K^* \Phi(\mathbf{f})] &= \sum_{y \in \mathcal{Y}} \mu K(y) \cdot \overline{\text{tr}} [K^* \Phi \circ \mathbf{f}(y)] \\ &= \sum_{y \in \mathcal{Y}} \mu K(y) \cdot \overline{\text{tr}} \left[\sum_{x \in \mathcal{X}} \frac{K(y|x) \mu(x)}{\mu K(y)} \Phi(\mathbf{f}(x)) \right] \\ &= \sum_{x \in \mathcal{X}} \mu(x) \overline{\text{tr}} [\Phi(\mathbf{f}(x))] \\ &= \overline{\text{tr}} \mathbb{E}_\mu [\Phi(\mathbf{f})] \\ &\geq \sum_{y \in \mathcal{Y}} \mu K(y) \cdot \overline{\text{tr}} [\Phi(K^* \mathbf{f})] \\ &= \overline{\text{tr}} \mathbb{E}_{\mu K} [\Phi(K^* \mathbf{f})]. \end{aligned}$$

Together with the fact that $\mathbb{E}_{\mu K} [K^* \mathbf{f}] = \mathbb{E}_\mu \mathbf{f}$ completes our claim. \square

APPENDIX B. CLASSICAL BONAMI-BECKNER INEQUALITY

In this section, we review the so-called *Bonami-Beckner inequality* in Theorem B.1. Consider the vector space of all functions $f : \{0, 1\} \rightarrow \mathbb{R}$ endowed with the inner product

$$\langle f, g \rangle = \frac{1}{2^n} \sum_{x \in \{0, 1\}^n} f(x)g(x) = \mathbb{E}[f \cdot g],$$

where we use the notation that the expectation is taken uniformly over all $x \in \{0, 1\}^n$. Then, every real-valued function defined on the Boolean hypercube can be uniquely expressed as the *Fourier-Walsh expansion*⁶:

$$f(x) = \sum_{S \subseteq \{1, \dots, n\}} \widehat{f}(S) \chi_S(x),$$

where the summation is over all 2^n subsets $S \subseteq [n] = \{1, \dots, n\}$ and

$$\chi_S(x) = (-1)^{\sum_{i \in S} x_i}$$

form an orthonormal basis (also called *Fourier basis*) since for any $S, S' \subseteq [n]$,

$$\langle \chi_S, \chi_{S'} \rangle = \begin{cases} 0 & \text{if } S \neq S' \\ 1 & \text{if } S = S'. \end{cases}$$

(We define $\chi_S \equiv 1$ for $S = \emptyset$.) Hence, for all $S \subseteq [n]$, $\widehat{f}(S) = \langle f, \chi_S \rangle$ is called the *Fourier coefficient* of f .

For any positive number γ , define T_γ to be

$$T_\gamma f = \sum_{S \subseteq [n]} \gamma^{|S|} \widehat{f}(S) \chi_S.$$

The well-known hypercontractive inequality states as follows.

Theorem B.1 (Bonami-Beckner Inequality [69, 72]). *Let $1 < p < q < \infty$ and let $\beta > 0$. Define $\gamma = \sqrt{\beta/(q-1)}$ and $\delta = \sqrt{\beta/(p-1)}$. Then for any function $f : \{0, 1\}^n \rightarrow \mathbb{R}$,*

$$(B.1) \quad \|T_\gamma f\|_q \leq \|T_\delta f\|_p,$$

where the norm is defined as

$$\|f\|_q = \left(\frac{1}{2^n} \sum_{x \in \{0, 1\}^n} |f(x)|^q \right)^{1/q} = (\mathbb{E}|f(x)|^q)^{1/q}.$$

By setting $\beta = p - 1$ and $q = 2$, the hypercontractive inequality (B.1) can be rewritten as

$$(B.2) \quad \left(\sum_{S \subseteq [n]} (p-1)^{|S|} \widehat{f}(S)^2 \right)^{1/2} \leq \left(\frac{1}{2^n} \sum_{x \in \{0, 1\}^n} |f(x)|^p \right)^{1/p}.$$

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⁶Some authors consider real-valued functions defined on $\{-1, 1\}^n$ with the Fourier basis $u_S(x) = \prod_{i \in S} x_i$. We note that either way of choosing the basis as 0/1-valued or \pm -valued does not influence the results presented in this section.

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